Catalytic combustion of liquid fuels

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Summary

This thesis discusses the use of catalytic combustion for liquid fuels, particularly unleaded petrol and diesel fuel. The intended application of this technology is for use in micro gas turbines, (typically 45 kW power output), which could be used to power the next generation of hybrid motor vehicles.

To perform this research a new test facility was constructed in the department of Chemical Engineering. The catalysts used were platinum and perovskite type ($LaMnO_3$), prepared experimentally. An industrially prepared platinum catalyst was obtained (Degussa), and used as a comparison.

Experiments were performed varying a number of key conditions (fuel type, catalyst inlet temperature, reactor pressure, fuel flow rate, and total mass flowrate), and results have been plotted graphically. Values for the observed reaction rate were then calculated.

As the reactor pressure increased, the observed reaction rate was shown to increase for all of the catalysts investigated and for both unleaded petrol and diesel fuel. As the fuel flowrate was increased the observed reaction rate was shown to increase for all the catalysts and both liquid fuels. As the total mass flowrate was increased the observed reaction rate was shown to increase for all the catalyst investigated and for both liquid fuels.

It was shown that the industrial Degussa catalyst had the highest activity for the catalytic combustion of diesel fuel, with an observed reaction rate of approximately $4x10^{-3}$ mol/s m^2. The perovskite catalyst showed the lowest activity, with an observed reaction rate of approximately $1x10^{-3}$ mol/s m^2; however, at high inlet temperatures the perovskite catalyst became comparable to the platinum catalyst, with an observed reaction rate of approximately $3x10^{-3}$ mol/s m^2 at an inlet temperature of 480°C.

When utilising unleaded petrol as the fuel the Degussa catalyst showed the highest catalytic activity with an observed reaction rate of approximately $7x10^{-3}$ mol/s m^2, with the platinum catalyst showing an observed reaction rate of approximately $4x10^{-3}$ mol/s m^2. The perovskite showed no activity for unleaded petrol.

The use of methane as a fuel was also investigated, however, none of the catalyst exhibited any activity across the range of catalyst inlet temperatures studied.

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This thesis, and all the work that has been performed to achieve it, would not have been possible without the continued support and funding from the EPSRC. The preparation of the experimental apparatus described in this thesis, was realised with the help of many individuals. I would like to personally thank all the Technicians in the Department of Chemical Engineering at the University of Bath for their total support and commitment to the cause, especially Mr Tony Comer, Mr Robert Brain and Mr Mac Forsyth. My heartfelt thanks goes out to you all. I would also like to thank the technicians in the Department of Mechanical Engineering for helping with some of the specialist equipment, particularly for the use of the analyser train.

During my period of studying I was fortunate enough to spend some time at the University of Naples and I would like to thank all concerned for the hospitality and good times that I had during my visit. I will also take a moment to thank all the friends that I made during my research period especially Mr Gareth Williams, and Miss Alexis Wilson for proving that research can be fun after all!

Finally I would like to especially thank my supervisor Prof. S. T. Kolaczkowski for his continued help and commitment to the research topic. Without his personal assistance this thesis could never have been written.

Nomenclature page:

A	Area	m^2
C_p	Constant pressure heat capacity	J/mol°C
D	Diameter	m
D_e	Hydraulic mean diameter	m
G	Mass flowrate	kg/s
m	Molar flowrate	mol/s
P	Pressure	bar
ΔP	Pressure drop	bar
r_{obs}	Observed reaction rate	$mol/s.m^2$
R	Universal gas constant	J/mol K
Re	Reynolds number	
T	Temperature	°C
U	Velocity	m/s
V	Volumetric flowrate	m^3/s
v_2	Volume per unit mass of fluid	m^3/kg

Greek symbols

ρ	Density	kg/m^3
μ	Viscosity	Pa s

Subscripts

1	Known conditions
2	Unknown conditions
o	Orifice
p	Pipe

Atmospheric pressure = ~ 1bar

Atmospheric pressure = ~ 20°C

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Chapter1: Introduction.

Combustion processes account for a large percentage of atmospheric pollution. Appendix A reviews the main pollutant species and their effect on the environment. In order to reduce this environmental impact, a cleaner combustion process is required - catalytic combustion.

One of the first observations of catalytic combustion can be found in the work of Sir Humphrey Davy 1818. He noted the sustained reaction of coal gas on a heated platinum wire without the formation of a flame. This phenomenon is now known as catalytic combustion.

Today catalytic combustion still utilises the same catalytic activity observed by Sir Humphrey Davy. The catalyst - the platinum wire in Sir Humphrey Davy's observation, has the effect of increasing the rate of reaction between fuel and oxygen, without the requirement of a flame.

1.1 The environmental benefits of catalytic combustion

It is well recognised that catalytic combustion can provide a cleaner primary combustion process [e.g., Dalla Betta *et al* 1994, Griffin *et al* 1994 etc]. Outlined below are some of the main environmental benefits of the technology.

1.1.1 NO_x Reduction

In conventional combustion, temperature profiles within the flame mean that the thermal NO_x formation temperature (1800 K [Zeldovich 1946, Saroffin and Flogan, 1976]) can be breached. As catalytic combustion does not require a flame, there is no temperature profile effect, and temperatures can be kept below the thermal NO_x formation temperature. This dramatically reduces NO_x emissions.

1.1.2 Reduction of carbon monoxide and unburned hydrocarbons

Catalytic combustion does not require near stoichiometric air to fuel ratios, unlike conventional combustion. Lean fuel mixtures, (usually outside the flammability limits), can therefore be utilised. This causes greater combustion efficiency, dramatically reducing the amount of unburned hydrocarbons in the exhaust stream. As the amount of available oxygen for combustion is greater, carbon monoxide emissions are also dramatically reduced.

1.1.3 Reduction of particulate emissions

Catalytic combustion has the potential to eliminate particulate emissions due to the extremely lean mixtures of air and fuel involved. In a standard stoichiometric combustion process, inadequate mixing and fuel rich regions can cause incomplete combustion. This can lead to particulate emissions. In the case of catalytic combustion, where the fuel and air are mixed together, a lean and uniform flow of reactants can be expected. This reduces the incidence of fuel rich regions, thereby minimising incomplete combustion and consequent particle generation.

1.2 Application to gas turbines

Over the last decade, activity in Europe, the US and Japan has increased in the race to resolve some of the fundamental problems in the development of a catalytic combustor for stationary gas turbines. Review papers on this topic are plentiful [e.g., Pfefferle and Pfefferle 1987, Kolaczkowski 1995, Johansson 1998, etc], a book describing the basic principles as well as advanced descriptions of specific features has also been published [Hayes and Kolaczkowski 1997]. Most of the work published and presented in the open literature has focused on large gas turbines (5-20 MW) for power generation [e.g., Ozawa 1994, Vortmeyer 1996 etc]. However, companies e.g., Volvo, Renault etc have been actively working on the development of small gas turbines both with and without catalytic combustors for the next generation of hybrid vehicles. The use of gas turbines in automobiles either alone or as a hybrid using "clean fuel" would drastically reduce tailpipe emissions particularly for inner city niche applications such as mass transportation vehicles and city trucks.

1.2.1 Description of a typical gas turbine

The theory of gas turbine operation is well documented, [e.g., Cohen *et al.* 1987 etc]. The gas turbine converts the chemical energy stored in a fuel into kinetic energy, with all moving parts being rotary. The principle of operation of a gas turbine is the basic Joule or Brayton cycle. The cycle comprises of four key energy exchange processes:

- Compression.
- Heat input.
- Expansion.
- Work output.

In a single stage gas turbine, a centrifugal or axial compressor compresses air from the atmosphere. This compressed air then enters a combustion chamber where fuel is injected and reacted with the oxygen from the compressed air. The high temperature and pressure products of the combustor are then expanded through a turbine producing enough power to drive the compressor and either power an external load (gas turbine), or produce thrust (Jet engine).

A simplified diagram of a single stage gas turbine is shown in *Figure 1.1*

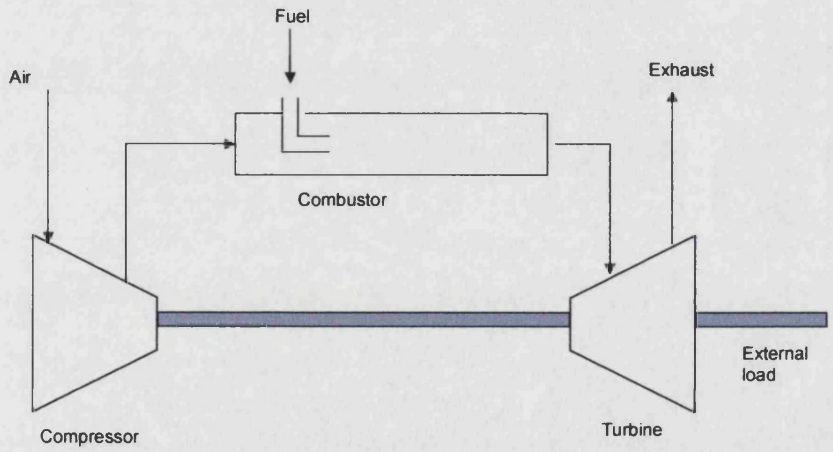

Figure 1.1: Simplified diagram of a single stage gas turbine

1.2.2 Operation of a conventional combustor

In a conventional gas turbine combustor, a flame accompanies the combustion of fuel. This type of combustion depends on free radical initiated oxidation reactions. In the combustion of hydrocarbons, these free radicals combine at a very fast rate with oxygen and fuel molecules, in a complex sequence of chemical reactions producing the final products of combustion, carbon dioxide and water. Other partial oxidation products including carbon monoxide, hydrogen, various hydrocarbons (e.g., aldehydes), etc., may also be produced. In a gas turbine, the heat released by these reactions can raise the final gas temperature from the combustor to 1800-2200 K [Trimm 1970, Zwinkels *et al.* 1993]. These high temperatures are well above the metallurgical limits for the turbine blades, as well as the thermal NO_x formation temperature. Addition of excess air is used to cool the combustion products so as not to damage the turbine blades.

The flame in a combustor can only propagate if the concentration of the combustible species is within the flammability or explosive limits [Chigier 1981]. The limits can be affected by the temperature and pressure of the air/fuel mixture, and by the presence of other species in the mixture, etc. For example, the lower and upper flammability limits for a mixture of methane in air at atmospheric pressure (~1.013 bar) are: 6.33 and 12.9 vol % of methane at 290 K and 4.8 and 16.6 vol % methane at 673 K [Spiers 1962]. The flammability limits for a great number of combustible species are well documented, e.g., [Lewis and von Elbe 1987].

The flame propagation constraint means that the excess air required to cool the combustor exit gases must by-pass the combustor. Unburned hydrocarbons and carbon monoxide can be formed in the combustor, due to incomplete combustion.

The operation of a conventional flame combustor is summarised in *Figure 1.2*

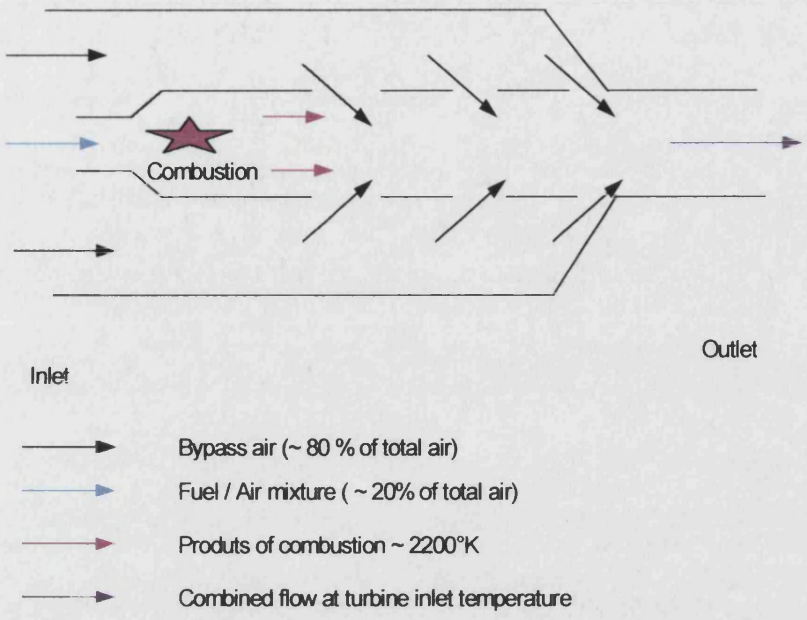

Figure 1.2: Operation of a conventional flame combustor

1.2.3 Operation of a catalytic combustor

In this type of combustor a catalyst is used to increase the rate of reaction without the formation of a flame. As flame stability is not an issue in this type of combustor, nor excess temperatures associated with flame combustion, there is no requirement for any air to bypass the combustion section. This results in leaner air/fuel mixtures in the combustion section. Also as catalytic combustion is not constrained by flammability limits, the fuel can be added to the air before the compressor section. This will ensure good mixing of air and fuel, and will reduce any fuel rich streamlines passing into the combustor, reducing the chances of catalyst hot-spots, and fuel remaining unburned. *Figure 1.3* shows the fundamental principles of a catalytic combustor.

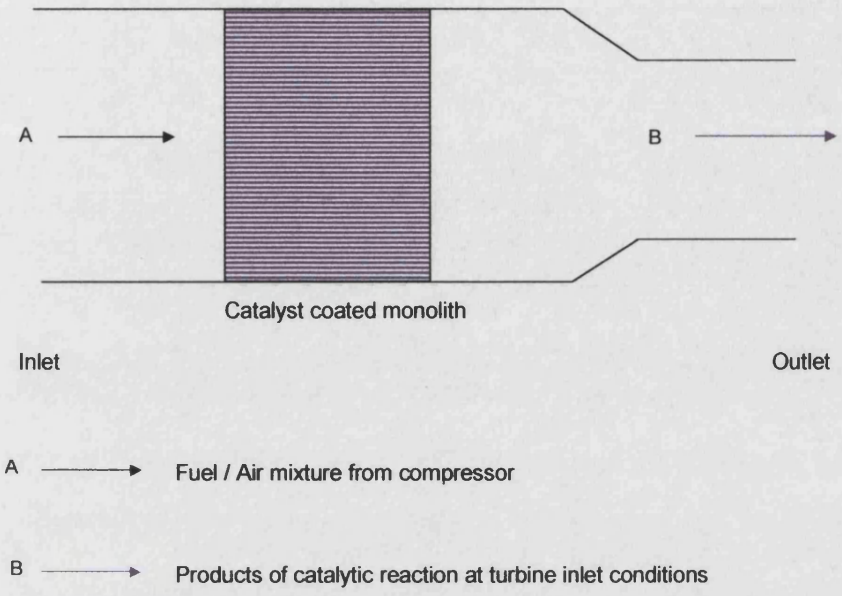

Figure 1.3: Operation of a catalytic combustor.

1.3 Aims of thesis

Few experimental studies have been performed using commercially available liquid fuels (petrol and diesel). The aims of this thesis are to study the catalytic combustion of these liquid fuels at conditions representative of a small gas turbine. This size of gas turbine is ideally suited for the automotive industry to power the next generation of hybrid vehicles. The use of petrol and diesel as fuels for these hybrid vehicles makes economic sense as a fully developed infrastructure already exists to supply them. The use of a catalytic combustor in the gas turbines of these vehicles could dramatically reduce any harmful emissions associated with conventional combustion.

1.3.1 Structure of thesis

The structure and order of this thesis begins with a literature review discussing the types of catalysts already used in catalytic combustion applications, how these catalysts are manufactured and how they can be characterised. This was used to select the catalysts that were produced for the experimental study. A chapter describing the apparatus used in the experiments is included detailing the main process units and analytical techniques used. Experimental procedures for manufacturing the selected catalysts and operating the main apparatus are also shown along with the experimental results and conclusions of the study. Finally a brief chapter on any future work to be performed leading directly from this investigation concludes the thesis. *Figure 1.4* shows the structure and order of the thesis

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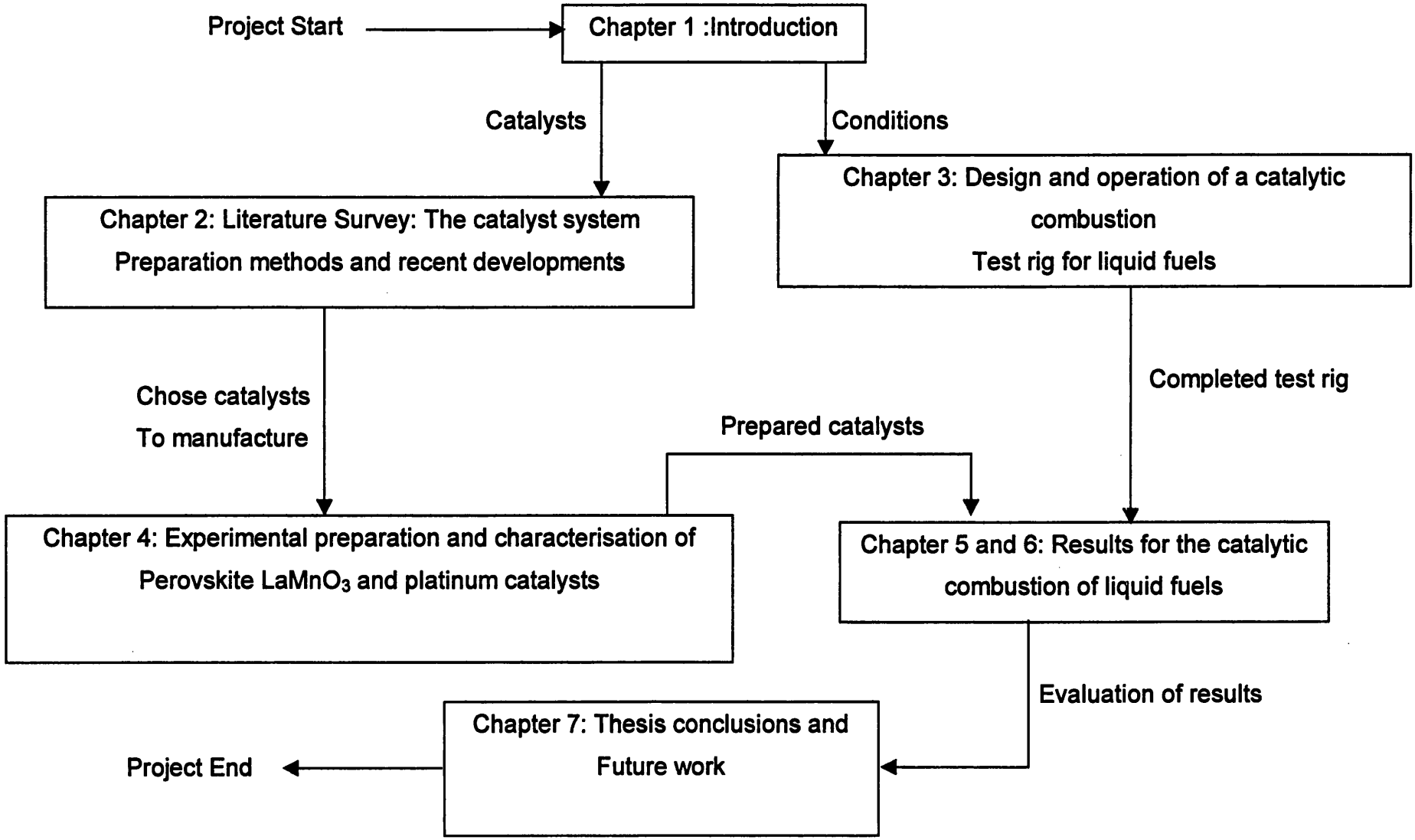


Figure 1.4: Structure and order of this thesis

Chapter 2 Literature survey: The catalyst system, preparation methods and recent experimental studies.

An enormous variety of substances exhibit catalytic activity of some type. Many of these, as studied in the laboratory in fundamental investigations, are prepared so as to have simple, uniform, or known structure rather than high area, high activity, or good mechanical strength. For an industrial catalyst the chemical composition is the most overriding consideration, but other factors, primarily of a physical nature, are usually also of major importance:

Surface area:	High surface area is usually desirable for high activity per unit volume or unit weight, so most catalysts are made to be porous, with internal surface areas ranging from about 10 m^2/g to as high as 1000 m^2/g. However the porous structure in the catalyst and pore size distribution may cause diffusional resistances that affect the rate and selectivity of the reaction. For very fast reactions like those associated with catalytic combustion a large pore size catalyst may be desired.
Stability:	This includes stability to heat (which is of key importance for catalytic combustion applications), to fluctuations in process conditions, and to such common components of reacting mixtures as water vapour. If a catalyst can be regenerated or reconstituted instead of being discarded, important savings may be realised, so stability to regeneration conditions may be important.
Mechanical properties:	Attrition resistance, hardness and compressive strength are of particular concern.

2.1 The catalyst system.

For catalytic combustion in gas turbine applications, the preferred support systems for the catalysts are monoliths. These have been developed over time based on their already popular application to catalytic converters. Most monoliths used today are made of either extruded cordierite ($2MgO.2Al_2O_3.5SiO_2$) – a low thermal expansion material that provides improved thermal shock resistance, or sintered metal (e.g., FeCrAlloy). Compared to ceramic monoliths the metallic ones are more durable towards mechanical stresses and vibrations, however, the maximum operating temperature is lower compared to some ceramic materials. Much research into the coating of metallic monoliths has been performed [e.g., Zwinkels *et al.*, 1994] but this is still more problematic than for ceramic monoliths.

The monolithic system enjoys several advantages over the traditional pellet systems, including lower pressure drop, and more rapid catalyst heat-up. In addition, monoliths, which have strong, thin, porous walls, are more durable than pelleted systems, since pellets become abraded with time. The millimetre-size parallel channels create a large surface area as well as being more cost effective than a pelleted system.

2.1.1 The washcoat.

Due to the low surface area of monolith substrates a high surface area coating is usually deposited upon its surface. This coating, known as a washcoat, provides a highly stable surface upon which the active phase of the catalyst can be dispersed. The washcoat layer can be manufactured from various materials, a selection of the most common being:

Alumina (Al_2O_3).

Alumina is one of the most common ceramics used in catalysis as a washcoat material, due to its high-temperature stability and large surface area. Alumina, which has a large specific surface area at temperatures below approximately 850°C, is not stable when submitted to higher temperatures. Due to dehydration, irreversible changes of the crystallographic phase can be observed as shown below in *figure 2.1* for Boehmite alumina.

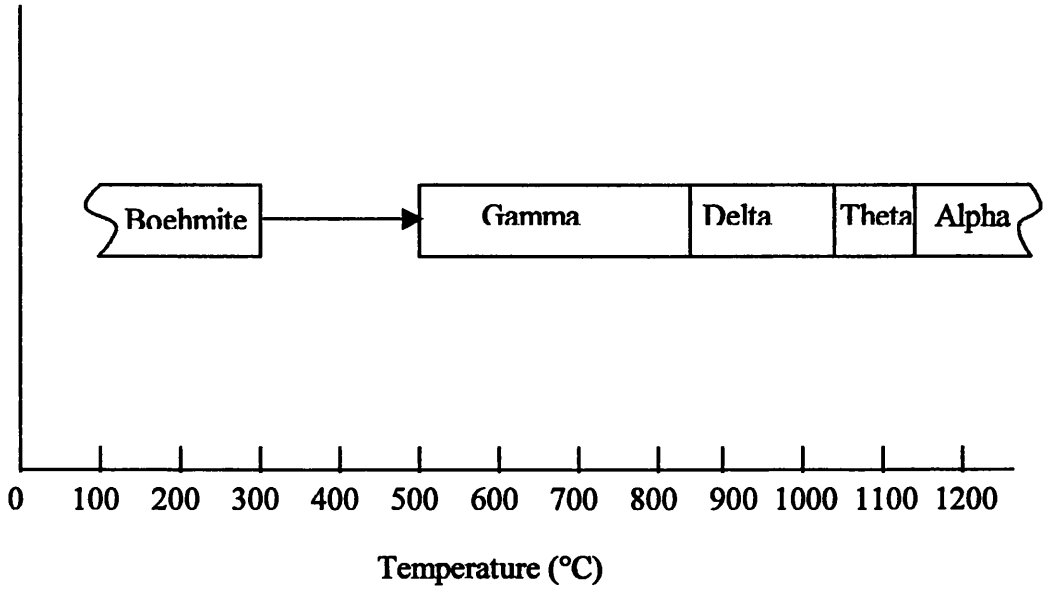


Figure 2.1: Decomposition sequence of Boehmite alumina. (Enclosed area indicates range of occurrence. Open area indicates transition range.) (Adapted from Wefers and Bell, 1972)

These phase changes lead to a sharp decrease in the specific surface area [e.g., Heck and Farrauto, 1995], however for applications below 850°C alumina is still the most widely documented material used for a washcoat material.

Magnesia (MgO).

Magnesia is also a possible washcoat material having a strong thermal stability. [Hashimoto *et al.* , 1991] describe a preparation by vapour oxidation, that can lead to a high surface area ultra-fine single crystal magnesia. It was shown to be very resistant to thermal treatment and had a surface area of 72 m^2/g after calcination at 1500°C.

Mulite ($3Al_2O_3 2SiO_2$).

The mulite structure has been observed by adding a high content of Si to alumina. [Arai and Machida, 1996]. The purpose of adding Si was to stabilise Al_2O_3 at temperatures above 1000°C. Mulite that retained a surface area of around 50 m^2/g after calcinating to 1300°C was produced by supercritical drying.

2.1.2 The active phase.

The most common active phases used in catalytic combustion applications are:

The platinum group metals.

Several of the elements of the platinum group metals have an outstanding capability in oxidising hydrocarbons, hydrogen and carbon monoxide. They have found widespread use as active materials in catalysts used at low to moderate temperatures. The high activity of the platinum group metals implies that they would be excellent candidates for use in gas turbine applications.

Due to their rarity and volatility at high temperatures, the use of the platinum group metals is limited to platinum, palladium and rhodium. Much research has been performed on these metals, and the activity of the platinum group metals in oxidation reactions is generally Ru<Rh<Pd<Os<Ir<Pt. [e.g., Prasad *et al.*, 1984].

The choice of metal is dependent on the fuel used. Platinum shows a high activity for oxidising carbon monoxide and saturated hydrocarbons (like those found in diesel fuel), while palladium is generally more active for partial oxidation of olefins [e.g., Trimm, 1991].

Palladium is the most common metal from the group used in catalytic combustion applications especially for natural gas or methane. At low

temperatures, the palladium is in the form of PdO_x. As the temperature increases there is a reduction of the PdO_x to metallic Pd at around 800°C. [Farrauto *et al.*, 1994, Quick and Kamitomai, 1995]. The reaction is reversible and the Pd-metal is re-oxidised back to PdO at 600°C in air. [Quick and Kamitomai, 1995]. It has been shown for natural gas and methane applications that metallic Pd is less active than PdO_x and much discussion has been concerned with the state of PdO_x that is most active, i.e. Pd with chemisorbed oxygen, Pd-particles with a skin of PdO of bulk PdO. [e.g., Burch, 1996, McCarty, 1995 , Kikuchi *et al.*, 1997, etc.]

The main problems in the use of platinum group metals, are sintering and evaporation at high temperatures.

Perovskites.

Perovskite-type oxides have the general formula ABO_3 where A is a large cation, usually a rare-earth ion (e.g., La, Pr, Nd, and Gd), and B is a cation, usually a transition metal ion. The B site cation is surrounded octahedrally by oxygen, and the A site cation is located in the cavity made by these octrahedra. The materials have a structure similar to $CaTiO_3$, which is the mineral that gave the name to the group, and are ideally cubic. A wide range of different perovskite-type materials have been manufactured, since almost 90% of the metallic elements in the periodic table could be substituted into the perovskite lattice. They have been found to be very promising catalytic materials, the catalytic activity and high thermal stability of the perovskites draw attention to their potential use as combustion catalysts. [e.g., Tejuca, 1989].

The catalytic activity of unsubstituted perovskite oxides for methane combustion has been studied [Seiyama, 1992]. It was shown that the activity was determined mainly by the B cation, the most active catalysts being those which contain Co or Mn in the B site. In a study looking at the influence of the A site cation on the catalytic combustion of methane, where the B site cation was fixed as Co [Baiker *et al,* 1993], no significant influence of the A site cation on the catalytic activity was found, with the exception of praseodymium which showed a 30 times lower activity than the other samples.

It is also possible to prepare more complex perovskites, giving rise to compounds of the type $(A_xA_{1-x})(B_yB_{1-y})O_3$. The partially substituted A and B sites could absorb and desorb large amounts of oxygen. This oxygen is more weakly bound

than the lattice oxygen [Ramesh et al., 1994]. Several types of substituted perovskites have been tested in combustion applications [e.g., Klvana et al., 1993, Baker and Metcalfe, 1995, Tsiakaras et al., 1998, Song et al., 1999, etc.], the cobalt, manganese and iron substituted perovskites all showing high activity.

Hexaaluminates.

These materials have the general formula $AB_xAl_{12-x}O_{19}$ where A could be an alkali, alkali earth, or a rare earth metal, and B could be a metal with similar size and charge as the Al ion. The two main features that have drawn attention to the use of hexaaluminates in catalytic combustion are resistance to sintering and a high catalytic activity. However the thermal expansion is high, hence hexaaluminates have a poor resistance to thermal shock. During the last decade a large number of different substituted hexaaluminate materials have been described, and the present state of hexaaluminates as combustion catalysts has been reviewed [Groppi et al., 1997].

Spinels.

The general formula of spinels is AB_2O_4. The A position represents a divalent ion such as Mg, Fe, Ni, Mn and Zn. The B position represents a trivalent metal ion e.g., Al, Fe, Cr and Mn. The spinal oxide has been described as a heat resistant material. Many different groups have studied the thermal properties and application in high temperature catalytic combustion [Lowe *et al.*, 1994, Marti *et al.*, 1994, Bolt *et al.*, 1995, Zwinkles *et al.*, 1998,].

Pyrochlores.

The pyrochlores are a group of compounds with the general formula $A_2B_2O_7$. They have been mentioned as materials for catalytic combustion applications [Ramesh *et al.*, 1994]. The A position can be a rare earth metal or an element with a lone pair of electrons, and the B position can be a transition metal. Several pyrochlores have been manufactured [Castro et al., 1989, Subramanian, 1990]. In a study of thermal stability of different complex oxides [Zwinkels et al., 1998], it was shown that after calcination to 1000°C the pyrochlore studied had a surface area of < 5 m^2/g. It was concluded that such materials are probably not suitable for high temperature applications unless the preparation method is improved.

Zeolites.

Zeolites are already widely used as catalysts for cracking applications and as shape-selective catalysts. The use of copper exchanged ZSM-5, ZSM-11 and ZSM-48 as well as Pd-ZSM-5 for propane and natural gas combustion was studied [Neyestanaki *et al.*, 1995]. Although the catalytic activity is good for the zeolite materials, the stability of the materials may prohibit their use in combustion applications.

2.2 Catalyst preparation techniques.

Catalysts are highly sophisticated products derived from chemicals by means of several different procedures. The catalytic properties are strongly affected by every step of the preparation together with the quality of the raw materials. Despite the variety of possibilities of preparing catalysts most can be reduced to a series of elementary steps, or unit operations. Such unit operations can be classified by:

1. The chemical and physical transformations, which are implied.
2. The scientific laws, which govern such transformations based on fundamental inorganic chemistry.
3. The operation variables such as temperature, pressure, pH, time, and concentration.
4. The general characteristics of the products of the operation.
5. The type of the required apparatus.

Most catalyst formulations involve a combination of some or even all these operations. However, even though the preparation procedures differ considerably from one catalyst to another, three broad categories can be introduced to classify the catalysts with respect to the preparation procedure:

1. Bulk catalysts.
2. Supported catalysts.
3. Mixed-agglomerated catalysts.

Most of the catalysts used in catalytic combustion are of the supported type, discussion of catalyst preparations will focus, therefore, on these types of

catalyst. For gas turbine applications the preferred supports are monoliths (section 2.1).

2.2.1 Manufacture of monoliths.

Most ceramic monoliths are manufactured by extrusion of thick cordierite dough through a die followed by drying and firing. A variety of cell shapes and sizes can be manufactured, and monolith blocks can likewise be fabricated in a variety of cross sectional shapes. Metallic monoliths are mainly manufactured by corrugation of thin metal sheets, which are spiralled around each other.

2.2.2 Addition of a washcoat.

A washcoat is usually added by dipping the blank monolith into a slurry containing the washcoat material. These slurries are a dispersed mixture of solid particles of metal oxides in water, and require constant agitation, as at rest the particles begin to floc together. The formation of flocs causes the slurry to become more viscous, and on occasion become solid like. This phenomenon is known as thixotropy. During the initial filling of the monolith channels, part of the water contained in the slurry is absorbed by the porous monolith walls. As a result, a coating in the form of a filter cake develops. The thickness of this cake is dependent on the substrate porosity and dimensions, slurry properties, and rate at which the channels are filled. The remaining coating load results from clearing the channels by blowing excess slurry out with air. The amount of coating deposited by this step is known to be a function of the air velocity and hence is dependent on the pressure driving the excess slurry from the channels [Kolb and Cerro, 1991].

After removing the excess slurry from the channels the monoliths are slowly dried and fired to solidify the coating to the channel walls without cracking or plugging.

2.2.3 Addition of an active phase.

Once the washcoat has been deposited on the support, there are two common methods for adding the active phase:

Precipitation.

In precipitation, the objective is to achieve a reaction of the type:

$$\text{Metal salt solution} + \text{Support} \xrightarrow{\text{Alkali}} \text{Metal hydroxide or carbonate on support}$$

The choice of the salt or alkali depends on many factors e.g., temperature and pH. The support is dipped into a slurry containing an amount of salt sufficient to give the required loading. Enough alkali solution is added to cause precipitation, and the catalyst is then removed and dried before being activated by calcination, reduction or other appropriate treatment.

Impregnation.

The impregnation method involves three steps:

1. Contacting the support with the impregnation solution for a certain period of time
2. Drying the support to remove embedded liquid.
3. Activating the catalyst by calcination, reduction, or other appropriate treatment.

Two methods of contacting the support with the impregnating solution may be distinguished, depending on the total amount of solution:

1. With excess of solution: The support is placed on a screen and dipped into excess quantities of solution for the time necessary for total impregnation. The catalyst is then drained and dried.
2. With repeated application of solution: This gives a more precise control, often termed dry impregnation or impregnation to incipient wetness. The support is contacted with a solution of appropriate concentration, corresponding in quantity to the total known pore volume. The catalyst is kept in motion in a rotating cylinder or drum, and is sprinkled as required with a solution of salt by sprayers. The disadvantage is the poorer distribution of precursors.

2.3 Recent developments of catalytic combustion applicable to gas turbines.

Researchers around the world have been trying to develop a catalytic gas turbine combustor. However as reported in a recent review article by [Kolaczkowski 1995], no commercial unit has been developed as fundamental problems in designing a catalytic combustor with industrial compatibility have yet to be resolved.

The basic principles of catalytic combustion and the development of the technology to gas turbine applications are well documented, especially in a number of review articles on the topic [e.g., Trimm 1993, Trimm 1991, Kesselring 1986, Pfefferle and Pfefferle 1987, Ismagilov and Kerzhentsev 1990, Zwinkels *et al.* 1993, Kolaczkowski 1995]. A number of additional papers describing theoretical and experimental studies on catalytic combustion for gas turbine applications have also been published in the literature. Groppi *et al* [1995a, 1995b] tested various mathematical models and evaluated their credibility in simulating homogeneous and heterogeneous reactions in a catalytic combustor. In a theoretical study, Kolaczkowski and Serbetcioglu [1996] demonstrated that it is not an easy task to evaluate chemical kinetic expressions at conditions which truly represent even the first stage (e.g., at gas temperatures from 623-973 K) in a catalytic gas turbine combustor, for as reaction rates become very fast, interphase and intraphase transport limitations also become significant. Vortmeyer *et al* [1996] described an experimental study on a catalytic hybrid combustor, which was shown to be able to attain an overall combustion efficiency of over 99.9%. However, the authors admitted that further work was required to ensure low NO_x emissions could be achieved at high temperatures. Because of the complexity involved in conducting experiments under transient conditions, most of the experimental studies in the past were performed under steady state conditions. Hayes *et al* [1996] investigated the catalytic combustion of methane under transient conditions both experimentally and theoretically which could be used to simulate the performance of a catalytic monolith during start-up and shutdown or when the loading was changed. In a study on the catalytic combustion of methane, Kolaczkowski *et al.* [1996] found that a one-dimensional model which incorporated intrinsic chemical kinetics,

intraphase diffusion resistance and employed Sherwood and Nusselt numbers attributable to laminar flow in channels for the assessment of interphase resistances was consistent with experimental results.

The vast amount of research in the field over the last two decades indicates that there is still a growing interest in the development of a commercial catalytic gas turbine.

Examples of experimental studies applicable to catalytic gas turbine combustors are presented in *Table B.1* in Appendix B.

Chapter 3: Design and operating procedures of a catalytic combustion test rig for liquid fuels.

To investigate the catalytic combustion of liquid fuels for the application of small gas turbines for uses in the automotive industry, a new experimental test rig was constructed.

3.1 Design Criteria.

To establish the design criteria the following key issues were addressed:

3.1.1 Fuels to be investigated.

As discussed in chapter 1, the application of catalytic combustion in small gas turbines to power the next generation of hybrid vehicles could help reduce harmful tail-pipe emissions. The use of both petrol and diesel fuel in such combustors would make commercial sense as a fully developed infrastructure already exists to supply these fuels.

As reviewed in Chapter 2, there are few examples of experimental studies investigating petrol and diesel as fuels for catalytic combustors, instead the majority of experimentation is based on methane or natural gas. This is because the foreseen market for catalytic combustion is in large stationary gas turbines used for power generation where the main source of fuel is methane or natural gas.

For these reasons, and to avoid the possibility of catalyst poisoning from any lead or sulphur components within the liquid fuels, the experimental test rig was designed to utilise unleaded petrol and low sulphur diesel as fuels. Provision was also included to allow reference experiments to be made using gaseous fuels e.g., methane.

3.1.2 Analysis considerations.

The evaluation of reaction kinetics can be complex even when a simple power law is utilised. Detailed discussion into the modelling of reaction kinetics can be found in a recent book [Hayes and Kolaczkowski, 1997].

In considering either petrol or diesel as fuels for a catalytic combustor, the evaluation of reaction kinetics would be particularly difficult. This is because both fuels are a combination of many different components. The compositions are also subject to seasonal changes, and may vary depending on where and from whom the fuels were brought.

To gain an understanding into the complexity of these fuels, samples of petrol and diesel were analysed using a Gas Chromatograph Mass Spectrometer (GCMS). The spectra produced were quantitatively analysed by BP Amoco LTD, a copy of the report is shown in Appendix C.

For the petrol sample, over 100 different compounds were uniquely identified as being present. The retention time of the sample in the GC was over 100 minutes. It was noted that the minor components above toluene could not be identified because of the presence of too many isomers.

For the diesel fuel only the quantities of normal alkanes were reported, and the retention time of the sample was over 40 minutes.

Clearly it can be seen that in order to perform an in-depth, detailed kinetic study of petrol and diesel combustion each of these components would need to be tracked across the catalyst. This would require sampling the inlet and outlet of the catalyst using a calibrated Gas Chromatograph (GC), (or other appropriate analysis technique), for at least 100 different components. The number of components is more likely to be far greater than 100 as during the catalytic combustion some of the larger components may crack to smaller new compounds, which would not have been detected in the inlet stream.

Even if a fully calibrated GC were available, based on the analysis performed by BP Amoco the sampling of petrol would take over 100 minutes for the inlet and 100 minutes for the outlet. This would require the catalytic combustion process to remain at steady state for 200 minutes for each of the conditions to be investigated.

For these reasons a detailed kinetic study of petrol and diesel combustion was dismissed as unfeasible. Instead, a total hydrocarbon content online analyser

(THC), was used to determine the total hydrocarbon content of the inlet and outlet streams enabling the amount of petrol and diesel combusted across the catalysts to be established.

3.1.3 Operating conditions.

An old diesel fuelled 45 kW Rover gas turbine was obtained by the department of mechanical engineering from the ministry of defence at Manadon. The operating conditions of this gas turbine are detailed in *table 3.1* below:

Flowrate of air through compressor	0.5 kg/s
Pressure ratio	2.8:1
Turbine inlet temperature	800°C
Theoretical thermal efficiency	6%
Heat exchanger	Non-Recuperated (no heat exchanger)

Table 3.1: Operating conditions of a 45 kW Rover gas turbine

The power output from this gas turbine is such that it is ideally suited for use in a hybrid vehicle application. Therefore, the main operating conditions were adopted and used as the design basis for the new test rig.

3.1.4 Catalysts to be studied.

As reviewed in chapter 2 platinum is a popular choice as a combustion catalyst, and has been shown to have a high activity in combusting saturated hydrocarbons. From the GCMS analysis of petrol and diesel it can be seen that they both contain a large number of these hydrocarbons. Little experimental data on this catalyst for liquid fuels can be found in the open literature, therefore this popular catalyst will be tested with liquid fuels.

Interest in the use of catalytic combustion for liquid fuels has been shown by a number of large industrial catalyst manufacturers, and a sample of an industrial catalyst designed specifically for diesel combustion has been acquired from Degussa. This catalyst is a cordierite monolith with a γ-alumina washcoat containing 90 g ft^{-3} (3178 g m^{-3}) of platinum as the active phase. This catalyst

will also be tested with liquid fuels and a comparison to the laboratory prepared platinum catalyst will be made.

Another group of catalysts that have been found to be promising for combustion applications are the perovskites. As detailed in chapter 2 the most active perovskites contain Co or Mn in the B site. Current research at the university of Naples in Italy is focussing on the perovskite $LaMnO_3$ for methane combustion, and laboratory production techniques have been refined to enable the active phase to be impregnated into a γ-alumina washcoat on a monolith support. No experimental data can be found in the open literature regarding the use of $LaMnO_3$ for the combustion of liquid fuels, therefore this catalyst will be tested in the new experimental test rig and the performance will be compared to the laboratory and industrially prepared platinum catalysts.

3.2 Test rig design.

The main test rig was manufactured making use of existing equipment from previous studies performed at the University. The following describe the main units used in the test rig:

3.2.1 Air supply .

The main air supply to the test rig is delivered from an air compressor capable of supplying a maximum of 1000 litres/min (0.0198 kg/s) of air at atmospheric pressure. The compressor stores air at 10 barg in an air receiver located in an outside store. Let-down air is supplied from the receiver to the test rig via a diaphragm let-down valve. The maximum air flowrate is below the stated design flowrate of 0.5 kg/s (section 3.1.2). However in the Rover gas turbine the size of catalyst that would be used to power the combustor is expected to be a standard industrial sized 4-inch (0.1016 m) diameter catalyst. The mass flowrate of air per unit area of catalyst is therefore approximately 60 $kg/s.m^2$. To obtain the same value of flowrate of air per unit area of catalyst in the test rig, the reactor section was fixed at a size of ¾ inch (0.01905 m)

3.2.2 The pre-burner.

In the design of the new catalytic combustion test rig, the pre-heater must be considered. This is required to produce the temperatures needed to reach catalyst light off, explained in detail in a recent book [Hayes and Kolaczkowski, 1997]. From the literature (Appendix B), most forms of pre-heater are either direct electric heating, or gas fired pre-burners. Use of a gas fired pre-burner involves flame combustion and would produce some emissions of nitrous oxides and carbon monoxide which could mask any of the emissions benefits gained from using catalytic combustion, furthermore the burner design would be complex as the test rig is designed to operate at pressure. A direct electric pre-heater was therefore the preferred solution. From literature and preliminary experimentation the catalyst light-off temperature is a function of the fuel used [Kolaczkowski, 1995]. It has been shown that methane has the highest catalyst light-off temperature typically 400°C. The electric pre-heater must therefore be able to heat the air supply to at least this temperature. The duty of the air heater was calculated as shown:

The maximum mass flowrate of the air supply = 0.0198 kg/s (1000 litres/min).
From the literature [Felder and Rousseau 1986] the heat capacity of air at atmospheric pressure is given by:

$$C_P = 28.94 + 4.15 \times 10^{-3} T + 3.19 \times 10^{-6} T^2 - 1.97 \times 10^{-9} T^3 \quad \text{J/mol°C.} \qquad (1)$$

Where T = Temperature (°C)

The air needs to be heated from atmospheric temperature (~20°C) to the catalyst light-off temperature of Methane (~400°C)

$$\text{Maximum duty of air heater} = m \int_{20}^{400} C_P dT \qquad (2)$$

Where m = Molar flowrate of air

= Mass flowrate/Molecular weight = 0.684 mol/s.

$\Rightarrow$ Maximum duty required $\approx$ 7.8 kW.

A 7.5 kW three phase electric heater was purchased from Leister, a division of Watlow. The heater was rated for atmospheric pressure use only, and included a Eurotherm feed back temperature controller. The controller measured the temperature of the air upstream of the heater and varied the power supplied to the heating coils according to the difference between the actual and set-point temperatures. To avoid burnout of the heating coils the temperature set point was increased gradually in increments of 50°C until the desired temperature had been achieved. The air flowrate through the test rig was constrained to a maximum of 750 litres/min, to avoid running the air heater to its maximum power limit.

As the electric heater was only rated for use at atmospheric pressure, it was necessary to consider a method to enable it to be used at the operating pressure of the test rig (section 3.1.2). Purchasing a second hand pressure vessel, certified to 10.5 bar, and attaching the heater inside achieved this. During operation the differential pressure across the heater was zero, as the difference in pressure between the rig and atmosphere was between the pressure vessel and the laboratory. The electric supply cables and controller cable were introduced into the pressure vessel through small holes in the vessel casing. These were then epoxy sealed from both the inside and outside ensuring a pressure tight seal.

Because the entire heater was locked inside the pressure vessel any stagnant air between the heater and the pressure vessel walls would pick up the heat losses from the heater casing. The electronics of the heater were delicate requiring a temperature less than 40°C to function correctly. To overcome this the air supply to the pressure vessel was from the front. This meant that cold air travelled over the outside casing of the heater to reach the air supply nozzle of the heater situated at the rear. As well as ensuring the average temperature inside the pressure vessel was as low as possible, supplying the air from the front of the pressure vessel enabled the air to be pre-heated before entering the electric heater, thereby reducing the duty required by the heater. A schematic of the electric heater design is shown in figure 3.1 below:

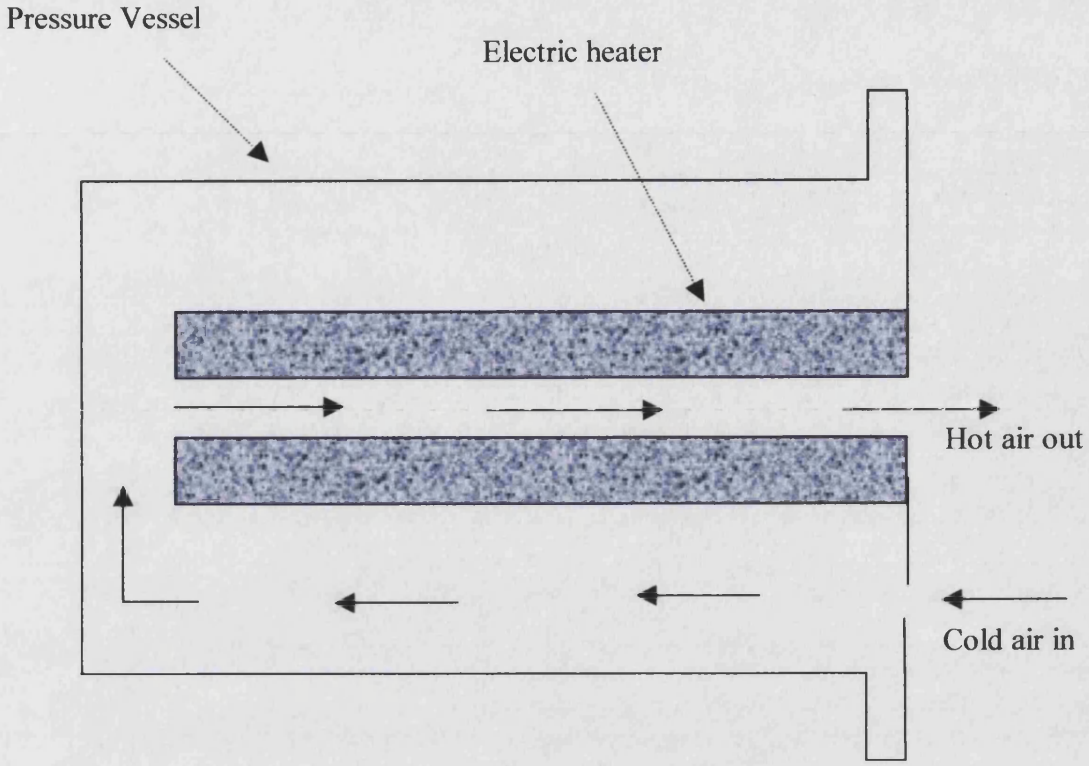


Figure 3.1: Schematic of the electric pre-heater design

3.2.3 Piping design.

Existing 2-inch mild steel pipe was used to supply the air from the receiver to the inlet of the electric pre-heater. As the outlet of the electric pre-heater was 4-inch (0.1016 m) and the catalyst reactor section had been designed as ¾ inch (0.01905 m), a stainless steel reducer in the shape of a cone was developed. The cone was designed and manufactured in house from off-cuts, the inclination angle was kept as low as possible to minimise any pressure drop effects. All of the pipework after the electric pre-heater was required to withstand temperatures up to 800°C, standard ¾-inch (0.01905 m), 316 stainless steel piping from Swagelok was used for this purpose, and all joins and connections were Swagelok compression fittings. A speciality back-pressure valve capable of withstanding the extreme temperatures, and a pressure relief valve set to lift at 5 barg were also purchased from Swagelok, and installed down-stream of the main catalyst reactor section. The entire test rig from the pre-heat to the exhaust gas clean up catalyst was lagged using high temperature fibre lagging.

3.2.4 Orifice plate design.

The flowrate of the air supply to the test rig needs measuring. This was achieved by the use of an orifice plate. The orifice plate was placed in the 2-inch pipework, before the electric heater, with the minimum length of straight pipe before and after the plate set at 14 pipe diameters. [Shell Handbook, 1993]. In order to calibrate the orifice meter a rotameter was installed. The orifice plate was designed as laid out below and manufactured in-house to the current British Standard:

Mass flowrate supplied from compressor = 0.0198 kg/s

Temperature of air stream through orifice ≈ 20°C

Recovery pressure ≈ 3 bar

From empirical formula [Perry 1984]:

Density = 3.57 kg/m^3.

Viscosity = 1.83×10^{-5} pa/s.

Volumetric flowrate through orifice plate = 5.56×10^{-3} m^3/s

Diameter of pipe = 2 inch = 0.0508 m

$$\text{Area of pipe} = \frac{\pi D_P^{\,2}}{4} = 2.03\times10^{-3}\ \text{m}^2$$

Estimate diameter of orifice = 0.4 inch = 0.01 m

$$\text{Area of Orifice} = \frac{\pi D_O^{\,2}}{4} = 8.11\times10^{-5}\ \text{m}^2$$

Velocity through orifice = 68.53 m/s

$$\text{Reynolds number through orifice} = \frac{\rho u D_O}{\mu} = 135928.$$

As Reynolds number is high assume coefficient of discharge (C_D) = 0.61

From orifice theory, and as the area of the orifice is small compared to the area of the pipe :

$$G = C_D A_O \sqrt{2\left(\frac{-\Delta P}{v_2}\right)}$$ [Coulson and Richardson Vol 1 1983]

Where:

G = Mass flowrate through orifice plate (kg/s).

A_O = Area of orifice plate (m^2).

ΔP = Pressure drop (Pa)

v_2 = Volume per unit mass of fluid = $\frac{1}{\rho}$ (m^3/kg)

$\Rightarrow$ $\Delta P = 22534$ pa = 0.225 bar.

This is a measurable pressure drop; therefore a 0.4-inch orifice plate was manufactured in house to the current British standards. The pressure drop across the orifice plate was measured using a differential pressure transducer, which was connected to the test rig following the British standards. The transducer was calibrated using a dead weight calibrator. The static pressure downstream of the orifice plate was also measured using a calibrated pressure transducer.

3.2.5 Fuel injection and mixing section.

The liquid fuels were pumped from a graduated 50 ml glass burette using a variable speed metering pump. The burette was filled with fuel when required from a 5-litre glass holding vessel. Methane was supplied to the test rig from a gas cylinder located in an outside store using a mass flow controller. If necessary, a nitrogen purge system was installed to purge the fuel lines. This was regulated using a second mass flow controller. Swagelok valves were installed to ensure that only one type of fuel could enter the test rig at any time via a common injection line.

To ensure quick and total vaporisation of the fuels, the common injection line was supplied directly into the hot air stream leaving the cone reducer after the pre-heater. Tightly wound stainless steel gauze was fitted inside the end of the line, protruding half way into the air stream. The hot air heated the gauze, which has a large surface area in contact with the fuel causing rapid and total vaporisation as the fuel passes through the gauze and into the rig.

To ensure homogeneous mixing of the fuel with the air an in line static mixer was manufactured. This consisted of many linked stainless steel quarter circle

baffles, which were fixed inside the ¾-inch piping. These baffles force the air and fuel to keep diverting in course, hence ensuring good mixing. Straight lengths of pipe directly before and after the static mixer were installed to ensure a uniform flow distribution profile.

3.2.6 Catalyst reactor section.

To enable modelling of the catalytic combustion of the fuels, temperature measurements before and after the catalysts were required. Wall temperatures of the catalysts were also required. These measurements were made using K type thermocouples connected to a data acquisition card on a PC. The thermocouples were fixed into the test rig using compression fittings, and were calibrated in ice and boiling water to ensure accuracy. Sample lines from the inlet and outlet of the catalyst reactor section were also installed, these joined a common sample line feeding the THC analyser, and a valve was used to switch between sampling the inlet and outlet. To avoid any hydrocarbons from condensing, the entire length of the sample lines were electrically traced and lagged to maintain a temperature inside the lines of approximately 200°C.

To record the pressure inside the test rig an electronic pressure transducer was installed into the test rig downstream of the main catalyst reactor section, this was calibrated using a dead weight calibrator.

3.2.7 Exhaust gas clean up catalyst.

After the main catalyst section, the exhaust gases will contain some unburned hydrocarbons, especially for low conversions through the main catalysts. An exhaust gas clean up catalyst was installed to completely combust any of these hydrocarbons. To ensure complete combustion of these hydrocarbons, the exhaust gases from the main catalyst section were expanded from the ¾-inch pipework to 4-inch. This expansion reduces the velocity of the exhaust stream, giving a longer residence time through the palladium based clean up catalyst.

3.3 Summary of catalytic test rig design.

The following flow diagram (Figure 3.2) shows the basic flowsheet of the completed test rig. A description of the components follows in table 3.2

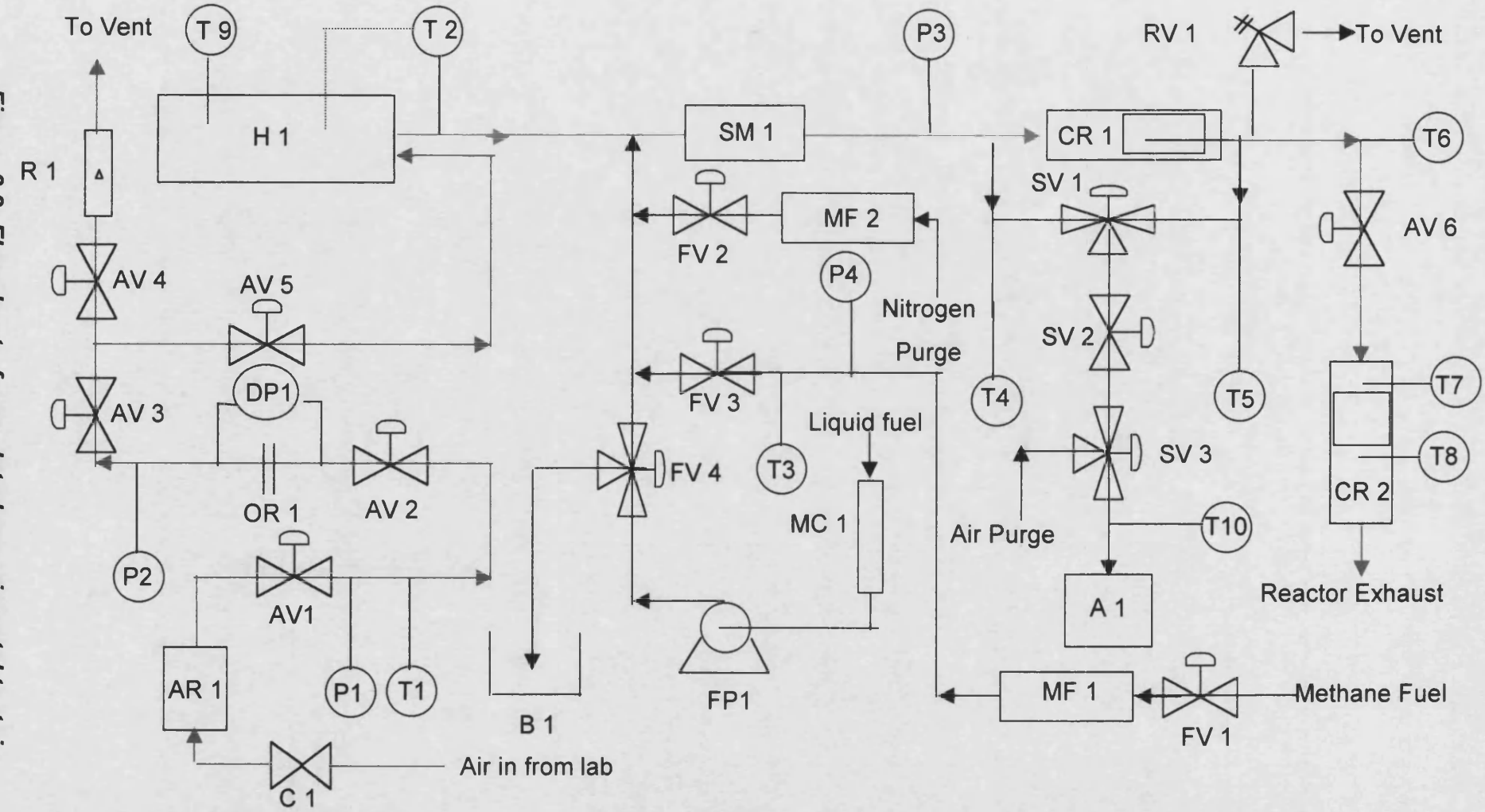


Figure 3.2: Flowsheet of completed experimental test rig

Equipment name	Description	Purpose
AV1	Air valve	Let air from the receiver into the test rig
AV 2	Diaphragm Air valve	Regulate air flow into test rig
AV 3	Air valve	Force a back pressure through the orifice plate
AV 4	Air valve	Divert air flow through rotameter
AV 5	Air Valve	Divert air flow through to the electric pre-heater
AV 6	Speciality Back pressure air valve	Force a back pressure through the test rig
FV 1	Fuel valve	Open methane to mass flow controller
FV 2	Fuel valve	Open nitrogen purge to test rig
FV 3	Fuel valve	Open methane to test rig
FV 4	Three way fuel valve	Either let fuel into rig or divert fuel into a collection beaker
SV 1	Three way sample valve	Allow sampling from either the reactor inlet or outlet
SV 2	Sample valve	Adjust flow of sample to analyser
SV 3	Three way sample valve	Allow analyser to sample either from the test rig or an air purge
P 1	Pressure gauge	Main air supply pressure
P 2	Pressure transducer	Static pressure upstream of orifice plate

Table 3.2: Description of the components in the test rig

Equipment name	Description	Purpose
P 3	Pressure transducer	Main reactor pressure
P 4	Pressure Gauge	Methane supply pressure
T 1	K Type thermal couple	Main air supply temperature
T 2	K Type thermal couple	Air temperature upstream of pre-heater. Used by controller to adjust duty of pre-heater
T 3	K Type thermal couple	Methane supply temperature
T 4	K Type thermal couple	Catalyst inlet temperature
T 5	K Type thermal couple	Catalyst outlet temperature
T 6	K Type thermal couple	Catalyst wall temperature
T 7	K Type thermal couple	Exhaust gas clean up catalyst inlet temperature
T 8	K Type thermal couple	Exhaust gas clean up catalyst outlet temperature
T 9	K Type thermal couple	Pressure vessel internal temperature
T 10	K Type thermal couple	Sample temperature entering analyser
C 1	Air compressor	Supply air for combustion experiments
AR 1	Air receiver	Receive and store air from compressor until required in test rig
OR 1	Orifice plate	Measure air flowrate
R 1	Calibrated air rotameter	To measure air flow at atmospheric pressure and temperature and to calibrate orifice plate

Table 3.2 Continued: Description of the components in the test rig

Equipment name	Description	Purpose
H 1	7.5 KW electric pre-heater inside pressure vessel	To heat air supply to the catalytic combustor
SM 1	Inline static mixer	Ensure fuel and air are mixed prior to entering catalytic reactor
CR 1	3/4 –inch Catalytic reactor	Contains the catalyst that combust the fuel
RV 1	Relief valve	To relieve test rig in case of over pressurisation
CR 2	4-inch Catalytic reactor	To combust any remaining hydrocarbons in the exhaust stream.
A 1	THC analyser	Analyse inlet and outlet of catalytic reactor for total hydrocarbons
MF 1	Mass flow controller	Regulate methane flowrate
MF 2	Mass flow controller	Regulate nitrogen purge
MC 1	50 ml Burette	Measure liquid fuel flow into the test rig
FP 1	Metering pump	Pump liquid fuel into the test rig
B 1	Plastic beaker	Collect liquid fuel when on bypass

Table 3.2 Continued: Description of the components in the test rig

3.4 Operating procedure.

The following procedure was used to operate the test rig safely:

3.4.1 Before starting any of the equipment.

The air, fuel and analysis streams have been flowsheeted (Figure 3.2). Before starting any equipment follow the flowsheet against the layout of the equipment in the lab. Check that all the valves are correctly labelled on the test rig and check that no modifications have been made.

3.4.2 Pre-Start up.

Before switching on any equipment ensure that the following checks have been performed:

1. Ensure AV1 is closed
2. Ensure AV2 is fully closed
3. Ensure AV3 is fully open
4. Ensure AV4 is open
5. Ensure AV5 is closed
6. Ensure AV6 is fully open

3.4.2.1 If liquid fuels are to be used:

Ensure the following checks are performed:

1. FV1 is closed
2. FV2 is closed
3. FV3 is closed
4. FV4 is in the position that sends fuel back to the collection vessel, rather than into the rig.

3.4.2.2 If Gaseous fuels are to be used:

Ensure the following checks have been performed:

1. FV1 is open
2. FV2 is closed
3. FV3 is open
4. FV4 is in the position that sends fuel back to the collection vessel, rather than into the rig.

3.4.3 Final checks.

1. Ensure SV2 is open
2. Ensure SV3 is in the position that sends air from the lab into the analyses. Rather than a sample from the rig.

3.4.4 Start up.

3.4.4.1Analysers.

The first pieces of equipment to start up are the analysers. They require approx. 1hr to warm up after first switching on. A detailed start up procedure for these analyses is supplied with the analysers. A brief summary procedure is as follows:

1. Plug the main sample line electric tracing control boxes in (the plugs are labelled T1 and T2)
2. Switch on the amplifier controlling the current for the top section of tracing and adjust to a value of approx. 70
3. Move the dial on the variac controlling the bottom section of tracing to a value of approx. 100. These settings should enable the temperature of the gas inside the traced sample lines to reach a temperature of approx. 180°C.
4. Switch on all 5 associated gas bottles
5. Switch on the pre-filter unit, HC analyser and NO_x analyser
6. Allow 30 minutes for equipment to heat up.

7. Check that the pre-filter display shows a temperature of approx. 180°C.
8. Use the *Status* and *Page up/down* buttons on the HC and NO_x analysers to check that the top three temperature values are not flashing. If they are flashing leave for a while longer.
9. Switch on the "Gold" bypass pump and the "blue" vacuum pump.
10. Press the *sample* key on both the HC and NO_x analysers to initiate the ignition process. The message "Prepare for sample" will be displayed on both analysers. Once ignition has occurred this will change to "sample"
11. Allow 30 minutes for the analysers to stabilise.
12. To calibrate the analysers press the *cal* button on both of the analysers.
13. If any technical or operational problems occur contact either Mr Alan Cox or Mr George Brunswick in the Department of Mechanical Engineering for advice.
14. Check the temperature of the gases in the sample line. Adjust the variac/amplifier if necessary.

3.4.4.2 Main control PC.

All necessary temperatures are recorded from the test rig to a display system on a PC. To access the programme

1. Switch on the PC
2. Upon seeing the dos prompt type "win"
3. When windows 3.1 has loaded open the program "Genie Builder"
4. When in Genie Builder open the file named "Main.prg" This is the program created to display all the temperatures etc that are measured directly from the tset rig.
5. Enter the run menu and scroll down to start. Type in a file name so the data can be stored on the computer hard-drive. If the data is to be exported to a spreadsheet package use a filename with a .prn extension.
6. Finally maximise the display window to view all the temperatures etc.

3.4.4.3 Air supply system.

While the analysers are warming up the main air supply for the catalytic combustor can be started:

1. Switch on the 3 phase supply box labelled "BOX 2".
2. Press the illuminated orange button on the air compressor. The orange light will go out.
3. Press the illuminated green button on the air compressor. This will start the compressor, and the pressure gauge located on the front panel will begin to increase.
4. Wait for the air pressure to reach 8 barg. The compressor will maintain this constant air feed pressure.

3.4.5 Steady state operation.

Once the analysers have had time to warm up, and have been calibrated, and the main air supply pressure of 8 barg has been reached, the following procedure can be used to run steady state catalytic combustion experiments:

1. Open AV1, the local pressure gauge should know read 8 barg
2. Start to open AV2 until a flowrate of air can be detected on the rotameter.
3. While closing valve AV3, and at the same time opening AV2, a know flowrate of air can be set on the rotameter at a fixed back-pressure through the orifice plate. For example a flowrate of 500 l/min of air (as stated by the rotameter) can be set for a back-pressure through the orifice plate of 5.0 barg. This system of measuring the air flow allows the main combustion section to be run at a constant air flowrate (evaluated at atmospheric pressure and temperature) for any desired pressure up to the set back-pressure (e.g. 5 barg) without having to change any air flow valves.
4. Once the desired air flowrate has been set, open AV5 and close AV4. This diverts the air through the main combustion test rig. At this point the air flowrate will be dictated solely by the values for the backpressure through the orifice plate and the actual delta P across the orifice plate. If either of these pressures change, adjustments to AV2 should be made to compensate.

5. Switch on the 415 volt supply labelled Box 1. A green and red display should be visible on the electric pre-heater control box. Use the up and down arrows to set the desired set point temperature. (If high temperatures are to be used a ramp of 100°C should be used)
6. Check to ensure the air is still flowing through the test rig (P2 and DP1 are still reading the set values)
7. Press the green button on the electric pre-heater control box. The red temperature should begin to rise.
8. Check all other temperatures (displayed on the PC) are rising accordingly.
9. Wait for steady state. **Do not leave the rig unattended while the electric pre-heater is on. It is also very important to keep checking that the airflow has not changed. Should the air flowrate drop to zero (i.e. P2 and Dp1 read zero or close to zero), the electric pre-heater must be immediately switched off by pressing the red button on the pre-heater control box.**
10. Adjust the reactor pressure to the desired value by closing AV6. **It is important to close this valve very slowly so as to minimise pressure waves through the test rig.**

3.4.5.1 Liquid fuels:

11. Once steady state has been reached switch on the main fuel pump (plug labelled FP1) and adjust the pump to give the desired fuel flowrate. Once this has been achieved divert the fuel flow into the test rig by switching FV4. A nitrogen purge can be achieved if required by opening FV2 and adjusting the appropriate mass flow controller.

3.4.5.2 Gaseous fuels:

11. Once steady state has been reached switch on the methane regulator (located on the cylinder in the outside gas store) and adjust to give a supply pressure greater than the pressure in the test rig (e.g. 6 barg). Use the associated mass flow controller to supply the desired fuel flowrate to the rig. If a nitrogen purge is necessary, opening FV2 and adjusting the appropriate mass flow controller can achieve this.

Important Note: Do not change from using a liquid fuel to using a gaseous fuel while the test rig is running. Switch off the rig and follow the whole procedure from the beginning.

12. Wait for all temperatures and pressures to reach steady state. (the main reactor pressure should be maintained by adjusting AV6 to compensate for any increase in pressure due to combustion).
13. Sample the reactor inlet by ensuring SV1 is pointing in the direction of the reactor inlet, and switching SV3 to allow the analysers to draw the sample. If the flowrate of sample is low/high (as indicated by the electronic rotameters on the front of both analysers) adjust SV2. Once sampling is complete switch SV3 back so that the analysers draw air from the lab
14. Repeat the sampling process for the reactor outlet, ensuring SV1 is pointing in the direction of the reactor outlet.

3.4.6 Shutdown procedure.

Once experiments have been finished, the test rig can be shut down by:

6. Turn off fuels
   Gaseous – Adjust mass flow controller to zero, and shut FV3 and FV1
   Liquid – Switch FV4 to divert fuel into collection beaker, pull plug FP1 out from Socket
7. Ensure any nitrogen purge is off, by adjusting the mass flow controller to zero, and shutting FV2
8. Fully open AV6
9. Press the red off button on the electric pre-heater control box, and use the down button to adjust the green temperature to 15°C. Switch 415 volt supply labelled Box 1 off.
10. Leave the air flowing through the combustor until all temperatures as displayed on the PC are below 100°C
11. Press the red button on the compressor control panel and switch the 415 volt supply labelled box 2 off.
12. Fully open valve AV3 and wait for the air receiver to empty.
13. Close valve AV1, AV2 and AV5 ready for next use.

14. Open AV4 ready for next use.
15. Turn off the electric tracing amplifier, and set the variac to zero.
16. Use the *page up/down* buttons on both the analysers until the stop command can be seen. Press the *stop* buttons on both analysers. They will then count down from 120 seconds and then display "standby"
17. Turn off the "gold" bypass pump, and the "blue" vacuum" pump
18. Turn off the analysers and the pre-filter unit.
19. Finally turn off all five related gas bottles.

3.4.7 Emergency Shutdown

In case of no airflow through the rig, P2 and DP will read approx. zero if this occurs SWITCH OFF THE FUEL FLOWS AS DESCRIBED IN THE SHUTDOWN PROCEDURES AND THEN HIT THE RED BUTTON ON THE ELECTRIC PRE-HEATER.

The rig has a pressure relief valve built in. It is currently set to lift at a reactor pressure of 5 barg. This can be adjusted in necessary. The valve relieves into the laboratory and will be very audible if it lifts. If the valve does lift OPEN AV6 IMMEADIATELY, SWITCH OFF THE FUEL FLOWS AS DESCRIBED IN THE SHUTDOWN PROCEDURES AND THEN HIT THE RED BUTTON ON THE ELECTRIC PRE-HEATER.

If the inlet temperature to the catalysts goes above the red temperature displayed on the pre-heater control box, the fuel is combusting homogeneously in the rig. SWITCH OFF THE FUEL FLOW AS DESCRIBED IN THE SHUTDOWN PROCEDURES AND THEN HIT THE RED BUTTON ON THE ELECTRIC PRE-HEATER.

If it becomes necessary to turn the air compressor off quickly, hit the big red button located on the compressor control panel. It is best not to have to shut the compressor off in this manor, especially if the electric pre-heater is on at the time. If the compressor has to be shut off in an emergency, it is essential that THE FUEL FLOWS ARE SWITCHED OFF AS DESCRIBED IN THE SHUTDOWN PROCEDURES AND THE ELECTRIC PRE-HEATER IS SWITCHED OFF.

Chapter 4: Catalyst preparations, characterisation and preliminary experimentation.

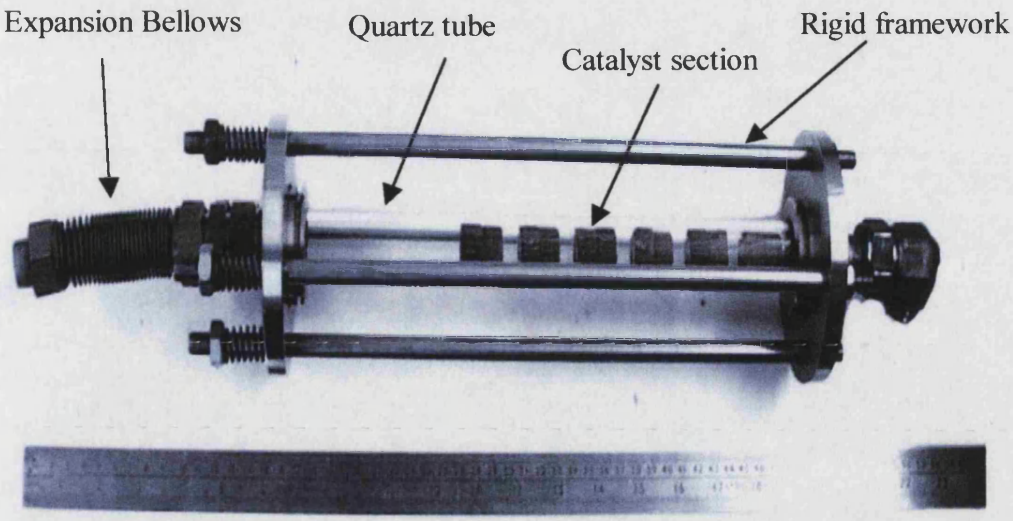
From the design criteria (chapter 3) perovskite and palladium catalysts were experimentally prepared, based on adapted techniques outlined in chapter 2. An industrial catalyst supplied by Degussa was also prepared. Before beginning the catalyst preparation the dimensions of the catalysts to use are required. These were experimentally determined by performing preliminary experiments

4.1 Preliminary experimentation to prove test rig operation.

To establish the dimensions of the catalysts to use in the main experiments and to prove the effectiveness of the fuel injection and mixing system of the test rig a few preliminary experiments were performed. The test rig was modified to enable visualisation of the catalysts in operation. This was achieved by replacing the ¾-inch reactor section with a 19 mm internal diameter quartz tube section. To prevent the delicate quartz from cracking due to expansion effects caused by the high temperatures, it was necessary to construct a rigid frame around the quartz tube. ¾-inch stainless steel expansion bellows were installed downstream of the quartz tube to absorb any stresses caused by the stainless steel pipework. The back-pressure valve was removed from the test rig, and the preliminary experiments were all performed at atmospheric pressure as the quartz tube would not withstand the high back-pressures.

Photograph 4.1 shows the construction of the quartz tube reactor section:

An old 4-inch palladium based catalyst was cut into 8 small cylindrical sections to fit inside the quartz tube each section being approx 20mm in length. The sections were kept apart inside the quartz tube using small sections of narrower diameter quartz tubing.

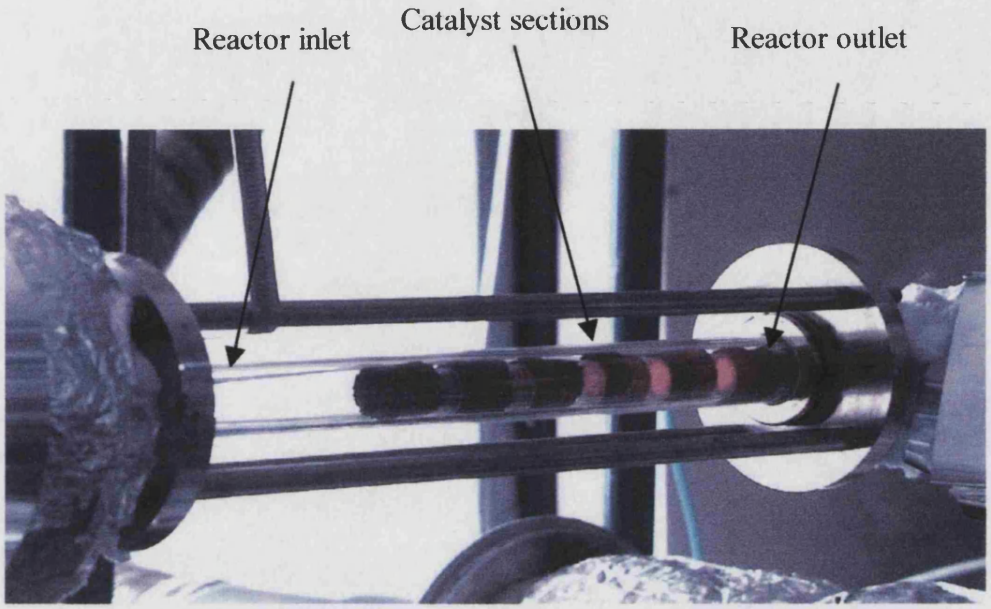


Photograph 4.1: Construction of quartz tube reactor section

The quartz reactor was installed in the test rig, which was run following the procedure outlined in chapter 3 section 3.4. The analysers were not used, as no quantitative information was required. The reactor pressure was atmospheric as the back-pressure control valve had been removed. The main air flowrate was set at 500 litres/min on the rotameter, and the pre-heater set point temperature was set to 400°C.

Once the test rig had reached steady state at 400°C, diesel fuel was introduced using the metering pump at a low flowrate. The actual flowrate used was not calculated, as no quantitative results were required. Visual inspection of the quartz tube as the fuel was switched on showed no signs of any liquid particles passing through the quartz reactor section. This proved the fuel injection system adopted, as all the diesel fuel must have been vaporised. Once the catalytic reactions had reached steady state, indicated by no further increase in the catalyst outlet temperature, the diesel flowrate was increased slightly. The flow of diesel was gradually increased until the steady state catalyst outlet temperature reached approximately 600°C. At this temperature the last couple of catalyst sections began to glow an orange colour. Visual inspection of the glowing catalysts showed the glow to be totally uniform across the whole catalyst diameter. This indicates that the inline static mixer must be performing well, as any fuel misdistributions would cause the orange glow to flicker across the catalyst

diameter. This is because at any point in time, some channels would see a fuel rich stream causing greater reactions and a brighter glow, while other channels would be subject to fuel lean conditions causing less catalytic reactions and a duller glow. *Photograph 4.2* below shows the catalysts glowing during the experimentation:



Photograph 4.2: Catalysts glowing during experimentation

Studying the catalysts it can be seen that the intensity of the orange glow of each catalyst section increased from the catalysts near the reactor inlet to the catalysts at the reactor outlet. The last two catalyst sections seemed to have a constant intensity glow. This can be explained as each catalyst section is performing a small percentage of the overall combustion, and the temperature of the reactant stream gradually rises as it passes from one catalyst section to the next. As the last two catalyst sections seemed to have the same intensity glow it can be surmised that these catalysts are performing no extra combustion. Therefore the first 5 catalyst sections are the only ones performing the combustion.

Each of the sections were approximately 24 mm in length therefore the total length of catalyst performing the combustion is 120 mm. This was used as the design basis for the manufacture of the main combustion catalysts.

4.2 Preparation of blank monolith support and the Degussa catalyst.

Industrial sized square channel, 4-inch (0.1016 m) blank monoliths were supplied from Degussa, containing 400 cells per square inch. A fully developed platinum coated monolith was also supplied to the same dimensions. The platinum loading of this catalyst was disclosed as 4 g platinum per litre of monolith.

The test rig reactor section was designed and manufactured from ¾-inch (0.01905 m) stainless steel (Chapter 3). The monoliths were therefore cut into appropriate sized cylinders. This was achieved using the nearest sized standard graphite corer, the monolith samples could only be cut to a depth of 0.02 m and the nearest corer gave a diameter of 0.015 m. The internal diameter of the ¾ inch (0.01905 m) reactor section was measured using callipers as 0.01885 m, the monolith sections therefore easily fitted inside the pipe, however a means of preventing the reactants from bypassing the channels and flowing around the gap between the monoliths and the pipe needed to be considered.

As the corer could only cut to a depth of 0.02 m, and from the preliminary experimentation the length of catalyst required was 0.120 m, 6 of these monolith samples gave the required length of catalyst for use in the test rig. A further monolith sample of each catalyst was manufactured for use in catalyst characteristic studies. This meant that for every finished catalyst 7 of the cored monolith samples were required.

4.3 Preparation of γ-alumina (Al_2O_3) Washcoat.

The use of γ-alumina as a washcoat was chosen because of its high surface area, and popularity (Chapter 2). As the maximum temperature of the test rig was designed to be 800°C (Chapter 3), the alumina would remain in the gamma phase and retain its surface area. The same washcoat was used for both the perovskite and palladium catalysts, and as the Degussa industrial catalyst also uses a γ-alumina washcoat, comparisons would be able to be made between the three different types of catalysts.

The required loading of the γ-alumina was fixed at 110g of γ-alumina per litre of monolith, as this is a common loading for combustion catalysts.

An adopted experimental procedure was followed, to produce an alumina/DISPERAL® suspension [Torncrona *et al* 1997].

Disperal® Boehmite (AlOOH) supplied by Condea Germany, was calcinated to 500°C for 3 hrs whereupon the boehmite was transformed into γ-Al_2O_3, with a quoted internal surface area of 160 m^2/g minimum. The resultant alumina was ground in a ball mill, and sieved through a 50 μm mesh, producing a powder with an average particle size less than 50 μm. A slurry was then prepared by dispersing 125 g of the alumina and 31.25 g of DISPERAL®, as binder in 457.5 g distilled water. Dilute nitric acid (11.5 g of 65 wt% nitric acid) was then added to lower the pH of the slurry, thus facilitating the dispersion of the alumina particles. The resultant slurry was continuously stirred using an overhead electric stirrer.

All of the required blank monolith samples were then dipped into the washcoat slurry for 1 minute, and then removed and left for 10 seconds. Excess solution was removed by blowing the channels with air, and the samples were then dried in an oven at 120 °C. the samples were then calcinated at 500 °C for 3 hours.

This procedure was repeated until the desired loading of approximately 110 g of γ-alumina per litre of monolith was reached.

To act as control experiments 7 washcoated monoliths were calcinated to 800°C for use in the test rig

4.4 Preparation of perovskite ($LaMnO_3$) supported on γ-alumina.

As defined in the experimental test rig design brief (Chapter 3), the perovskite $LaMnO_3$ was used for the catalytic combustion of liquid fuels. Current research at the University of Naples has shown that this perovskite shows good catalytic activity for methane combustion, however the catalysts are not as active as the platinum group metals. Perovskite catalysts were therefore manufactured with double the active phase loading of the Degussa catalyst i.e., 8 g $LaMnO_3$ per litre of monolith. To investigate the effect of the amount of active phase on the catalytic combustion, samples were also made containing triple this amount i.e., 24 g $LaMnO_3$ per litre of monolith.

The so-called Deposition-Precipitation route was used to deposit the active phase. Lanthanum and manganese hydroxides produced from lanthanum nitrate ($La(NO_3)_3 \cdot 6H_2O$, Fluka, > 99%), and manganese acetate ($C_4H_6MnO_4 \cdot 4H_2O$, Sigma, > 99%), were preferentially co-precipitated on the surface of pores in the washcoat. During calcination, these hydroxides break down, leaving the perovskite structure on the pores of the washcoat.

It is required to manufacture catalysts containing 8 and 24 g $LaMnO_3$ per litre of monolith. The solutions were prepared based on the higher 24 g $LaMnO_3$ case.

The amount of active phase to deposit in 110 g/l of washcoat is 24 g/l. The percentage active phase in the washcoat was therefore calculated as:

$$\%\ \text{Active phase in washcoat} = \frac{\text{Mass of active phase}}{\text{Mass of active phase} + \text{mass of washcoat}} * 100$$

$$= \frac{24}{24+110} * 100 = 18$$

⇒To produce 1 g of the final supported catalyst, 0.82 g of washcoat and 0.18 g Perovskite were required.

Molar masses:

Perovskite ($LaMnO_3$) = 241.86 g/mol

Manganese acetate ($C_4H_6MnO_4 \cdot 4H_2O$) = 245 g/mol

Lanthanum nitrate ($La(NO_3)_3 \cdot 6H_2O$) = 433 g/mol

Urea (CH_4H_2O) = 60 g/mol

⇒ Moles of perovskite required = 7.44×10^{-4}

1 mole perovskite requires 1 mole of lanthanum nitrate and 1 mole of manganese acetate.

⇒ Total moles of cationic species = $2 \times 7.44 \times 10^{-4} = 1.49 \times 10^{-3}$

Urea (CH_4H_2O, Fluka, >99.5 %) is used as a base to promote the co-precipitation of the hydroxides. Urea was added in the molar ratio urea/cationic species 9:1.

$\Rightarrow$ Moles urea required = 1.34×10^{-2}

$\Rightarrow$ Mass of lanthanum nitrate required = 0.323 g

Mass of manganese acetate required = 0.183 g

Mass of urea required = 0.804 g

Normalising to 1 g of washcoat

Require: 0.394 g of lanthanum nitrate

0.223 g of manganese acetate

0.980 g of urea

The volume of a single cored monolith sample to coat was given by:

Diameter = 15 mm (section 4.1)

Length = 120 mm (section 4.1)

$\Rightarrow$ Volume = 2.12×10^{-5} m^3 = 2.12×10^{-2} litres.

Estimating the total number of monolith sections to coat as 20 (14 sections were required but extra were manufactured)

$\Rightarrow$ Total volume = 0.424 litres.

The mass of washcoat deposited on the monoliths was 110 g per litre of monolith

$\Rightarrow$ Total mass of washcoat to deposit active phase in = 46.64 g.

$\Rightarrow$ Require: 18.376 g of lanthanum nitrate

10.401 g of manganese acetate

45.707 g of urea

The porosity of the γ-alumina washcoat was roughly estimated as 1 ml/g.

⇒ A solution of 46.64 ml containing 18.376 g lanthanum nitrate, 10.401 g manganese acetate and 45.707 g urea would deposit the required loading of the active perovskite phase in a single dipping.

The quantities of reagents required were large, and the solution volume was relatively small, therefore a 500 ml solution containing 1/3rd of the quantities of reagents was prepared, and the monoliths were dipped into the solution multiple times, until the desired coverage was achieved. Each dipping required the monoliths to be suspended in the solution for approximately 10 minutes. The solution was continuously stirred using a magnetic stirrer and maintained at 90°C on a hot plate with a reflux condenser to avoid evaporative losses. Under these conditions, the urea slowly decomposed producing ammonia homogeneously in the suspension, thus causing the preferential co-precipitation of hydroxides on the surface of pores in the support. Excess solution was removed from the monoliths by blowing the channels with air. The monoliths were then dried in an oven at 120°C, before being calcinated at 500°C for 3 hours. Once the required coverage had been achieved the catalysts were fixed by calcinating to 800°C for 3 hours.

4.5 Preparation of platinum catalysts supported on γ-alumina

As defined in the experimental test rig design brief (Chapter 3), platinum catalysts were to be manufactured and tested for the catalytic combustion of liquid fuels. To compare the prepared platinum catalysts with the industrial Degussa sample, the amount of platinum deposited in the washcoat should be the same i.e., 4 g platinum per litre of monolith. To investigate the effect of the amount of active phase on the catalytic combustion, samples were also made containing double this amount i.e., 8 g platinum per litre of monolith.

The preparation was based on depositing the required amount of platinum inside the pores of the washcoat. The source of platinum was Hexachloroplatinic (IV) acid (H_2Cl_6Pt, > 99.9%, Sigma-Aldrich), this was reduced in the pores of the

washcoat to metallic platinum using Hydrazine according to the following equation:

$$H_2Cl_6Pt_{(aq)} + N_2H_{4(aq)} \rightarrow Pt_{(s)} + N_{2(g)} + 6HCl_{(aq)}$$

As the hexachloroplatinic (IV) acid was expensive, a dilute aqueous solution was prepared by dissolving 2 g into 200 ml of distilled water. The solution was continually stirred using a magnetic stirrer.

The washcoated monoliths were placed in a plastic beaker and evacuated to 30 inches mercury in an evacuation jar for 30 minutes. This helped remove air from the washcoat pores enabling the Hexchloroplatinic (IV) acid solution to penetrate deep inside the washcoat. Once evacuated the Hexchloroplatinic (IV) acid solution was spayed into the monoliths still under vacuum conditions until the monoliths in the beaker were completely submerged. The monoliths were left in the solution and under vacuum for 30 minutes, after which they were removed and transferred to a second beaker. The remaining hexachloroplatinic (IV) acid solution was recycled to avoid wastage. Excess dilute Hydrazine solution was then added to the beaker until the monoliths were once again submerged. The monoliths were then left for 30 minutes, or until the nitrogen evolution was seen to have stopped.

To remove any hydrochloric acid present in the washcoat, the monoliths were washed with excess distilled water before being dried in an oven at 120°C before being calcinated to 500°C for 3 hours. This process was repeated until the desired platinum loading was achieved, after which the monoliths were fixed by calcinating to 800°C for 3 hours.

4.6 Catalyst characteristics

The following two characteristic techniques were performed to one of each of the finished catalyst sections:

1. BET surface area and pore size distribution analysis
2. Scanning electron microscopy analysis using a Philips 7020 electron microscope.

These techniques were kindly performed by the department of Material Sciences using an ASAP machine for BET surface area and a Philips 7020 for the SEM analysis.

4.7 Assembly of finished catalysts into the test rig.

The finished catalysts were assembled into the reactor section of the test rig as illustrated in *Figure 4.1* below:

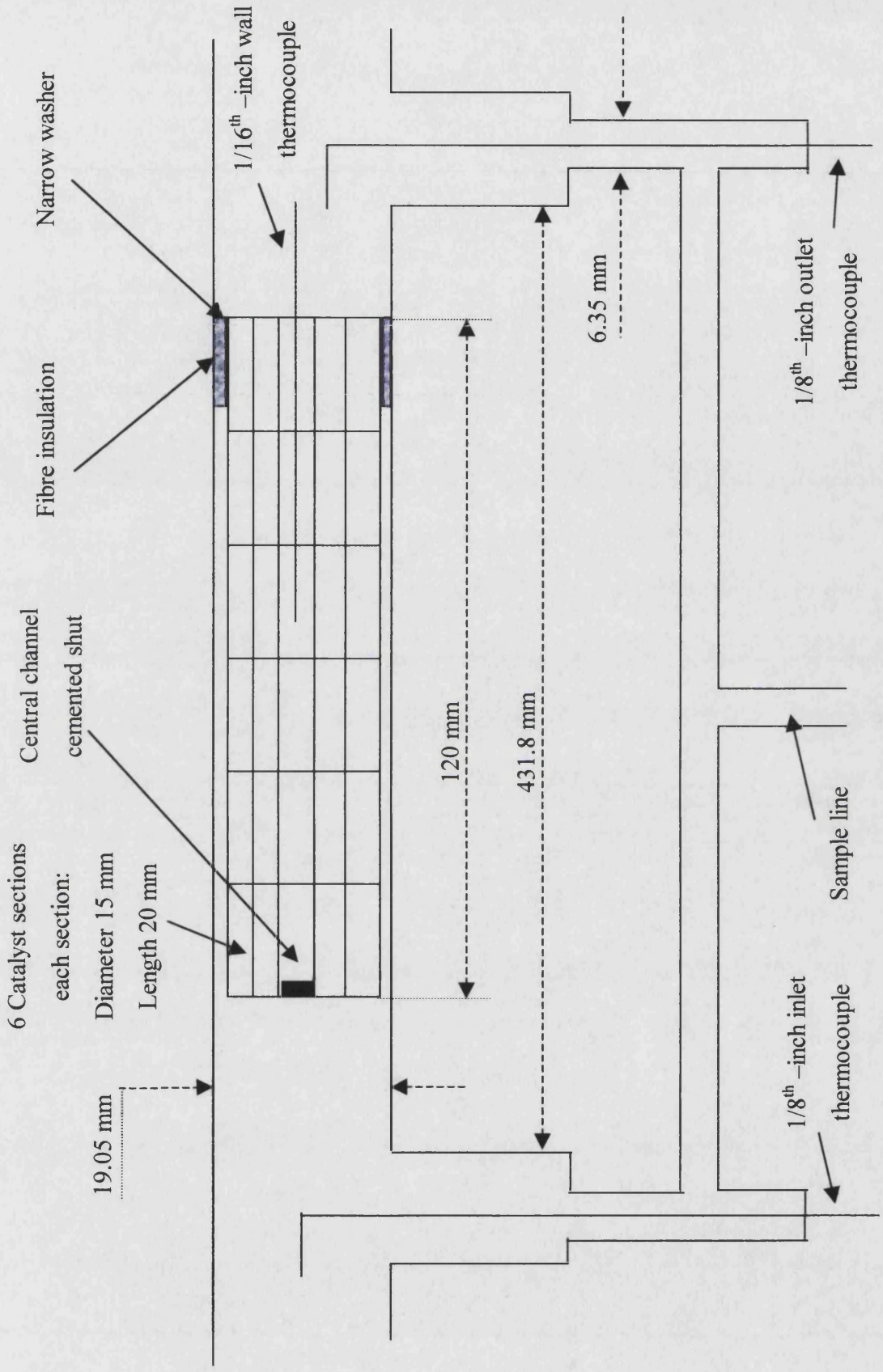


Figure 4.1: Assembly of catalysts into the reactor section of the test rig

A thin walled washer was manufactured from stainless steel and trapped between the compression fittings of the ¾-inch pipe and the reactor outlet T piece such that the catalysts could not be blown out of the test rig. To prevent any bypassing of the reactant stream around the outside of the catalysts between the catalyst wall and the pipe internal diameter, a small quantity of fibre insulation was also trapped between the compression fitting of the pipe and the reactor outlet T piece. When this fitting was tightened, the fibre insulation compressed around the last monolith, giving a tight seal. The central channel of the middle monolith section was fire cemented closed on the side nearest the reactor inlet. A thin wall thermocouple was then located into this central channel (through the back two monoliths), such that the thermocouple was approximately ¾ of the way inside the monolith from the reactor outlet side.

4.8 Fuel flowrates used for the combustion experiments.

The fuel flowrates used for the combustion experiments were obtained from adiabatic temperature calculations. The amounts of the three fuels (Unleaded petrol, Diesel and methane), to supply into the test rig were based on obtaining a temperature rise over the catalysts from an inlet temperature of 500°C to an outlet temperature of 800°C at total conversion. The following calculation shows how the flowrate of diesel to supply to the test rig was calculated:

Assumption: The fuel component in the air stream is small and can be ignored

Energy required to heat air from 500°C to 800°C

This was calculated from:

$$\text{Energy required} = m \int_{500}^{800} C_P dT$$

Where:

m = Molar flowrate of air (mol/s)

Cp = Heat capacity of air (J/mol°C)

T = Temperature (°C)

From the literature [Felder and Rousseau, 1986] the heat capacity of air is given by:

$$C_P = 28.94 + 4.15 \times 10^{-3} T + 3.19 \times 10^{-6} T^2 - 1.97 \times 10^{-9} T^3 \quad \text{J/mol°C.}$$

Where T = Temperature (°C)

The flow rate of air was taken as the design basis of 500 l/min at 20°C and atmospheric pressure.
Assuming air to be an ideal gas with a molar mass of 29 g/mol, the molar flowrate of air was calculated as 3.42×10^{-4} kmol/s

⇒ Energy required = 3.33 kJ/s

Energy released form the combustion of diesel fuel

The flowrate of diesel fuel was initially estimated as 10 ml/min at 20°C and atmospheric pressure. The density of the liquid diesel fuel was experimentally determined as 840 kg/m^3 at room temperature (~20°C), giving a mass flowrate of diesel into the test rig of 1.4×10^{-4} kg/s.
From data sheets on diesel [British Petroleum Company Limited] the net calorific value of diesel fuel was taken as 42374 kJ/kg.

⇒ Energy released from the combustion of the diesel = 5.93 kJ/s.

The calculation was performed in a spreadsheet enabling the energy balance between the energy released from the combustion of diesel fuel and the energy required to heat the air from 500°C to 800°C to be set to zero by changing the diesel fuel flowrate.

⇒ Flowrate of diesel required to satisfy energy balance = 5.6 ml/min

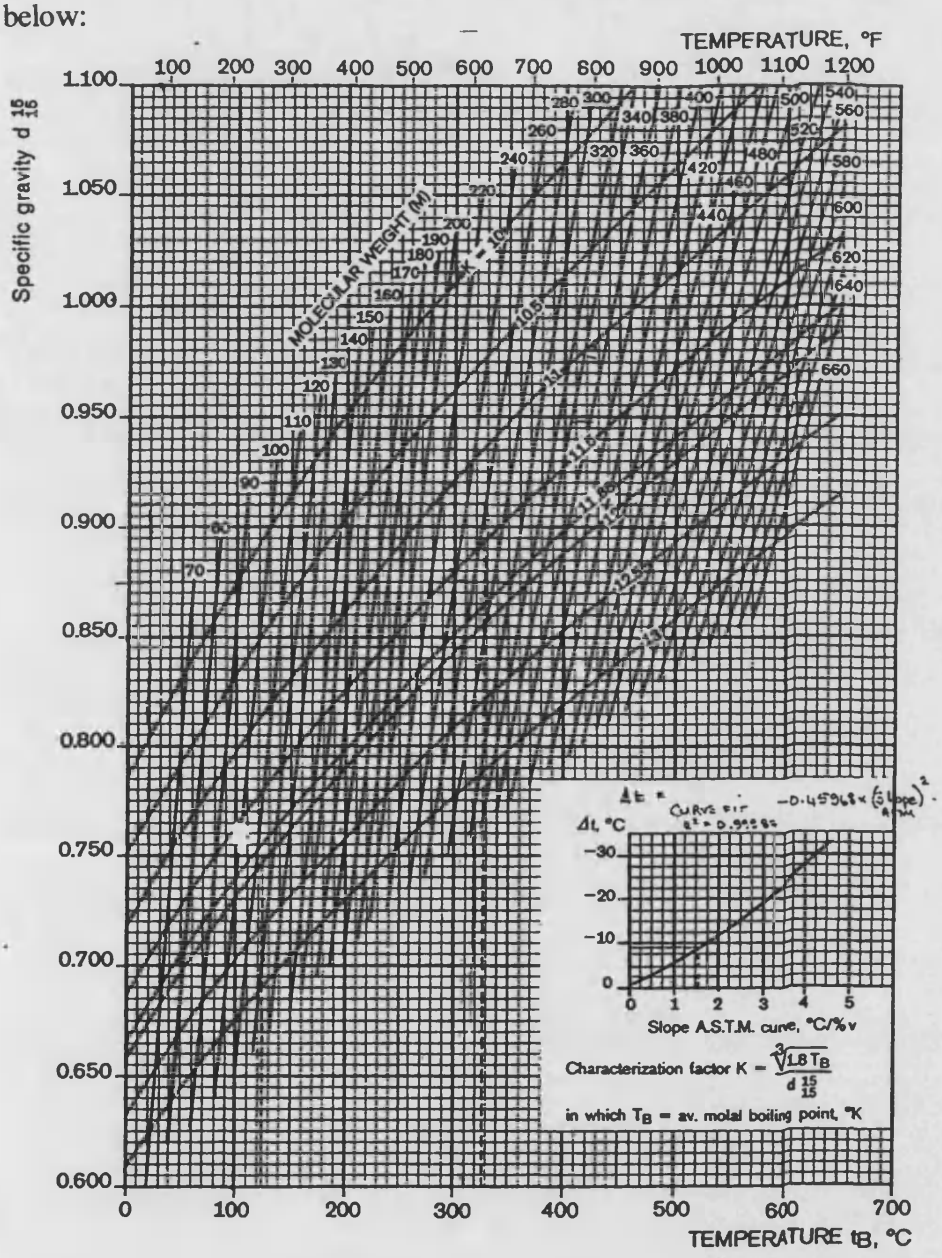
By a similar method the flowrates of unleaded petrol and methane were established as:

Unleaded petrol 6.1 ml/min

Methane 9 litres/min

4.9 Molar masses of diesel and unleaded petrol

The molar masses of diesel and unleaded petrol are required. These were obtained using a method described in the literature [The science of Petroleum, K.M. Watson]. The method calculates the molar masses of petroleum fractions from specific gravity and average molal boiling point using *Graph 4.1* included below:



Graph 4.1: Curves of molar masses of petroleum fractions plotted by specific gravity and average molal boiling point.

(Source: The Science of Petroleum, page 1379 Fig 2; K.M. Watson)

For diesel fuel the ASTM distillation range was obtained from data sheets [British Petroleum Company Limited] as:

10%	195°C
30%	226°C
50%	260°C
70%	298°C
90%	338°C

$$\Rightarrow \quad \text{Volume average boiling point} = \frac{10\% + 30\% + 50\% + 70\% + 90\% \text{ point}}{5}$$

$$= 263.4°C$$

The slope of the ASTM curve is given by:

$$\frac{338 - 195}{80} = 1.79$$

From *Graph 4.1* the correction Δt = - 10°C

$\Rightarrow$ Average molal boiling point = 263.4 - 10 = 253.4°C

The density of diesel fuel was determined experimentally as 840 kg/m^3 at room temperature (~20°C), giving a specific gravity of 0.84. From *Graph 4.1*:

Molar mass of diesel = <u>200 g/mol</u>

Using the same technique the molar mass of unleaded petrol was also obtained. The density of unleaded petrol was experimentally obtained as 733 kg/m^3 at room temperature (~20°C):

Molar mass of unleaded petrol = <u>98 g/mol</u>

Chapter 5: Results for the Catalytic Combustion of Unleaded petrol.

5.1 Results obtained using Platinum Catalysts.

Experiments were performed using platinum catalysts of fixed dimensions, with two different amounts of active phase. All monoliths had an initial gamma alumina washcoat layer of approx 112g alumina per litre of monolith, which were calcined to 500°C. The Platinum active phase was added to give finial catalysts with approx 4g Platinum per litre of monolith, and 8g Platinum per litre of monolith. Both finished catalysts were calcined to 800°C. Full details on the production of the catalysts can be found in Chapter 4.

5.1.1 Inlet Temperature effects.

In these experiments the effect of changing the catalyst inlet temperature on the catalytic combustion of unleaded petrol was investigated. All other conditions in the test rig were fixed. The platinum catalysts were assembled into the test rig as described in Chapter 4. The flowrate of air through the rig was fixed at 500 litres/min (Evaluated at 20°C and 1 bar pressure). The Unleaded Petrol was pumped into the test rig using a metering pump at a fixed rate of 6.1 ml/min, (Chapter 4), (Evaluated at 20°C and 1 bar pressure). The reactor pressure was fixed at 2 bar gauge using a back-pressure control valve. The catalyst inlet temperature was varied by altering the electric air heater set point from 350°C to 500°C in increments of 50°C. At each different temperature set point the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in Chapter 3. The experiment was repeated twice recorded as run 1 and run 2 respectively. The results can be found in Appendix D.

From the raw experimental results, values for the observed reaction rate were calculated as shown below:

$$\text{Observed Reaction Rate (mol/s.m}^2\text{)} = \frac{\text{Molar flow of Petrol Combusted}}{\text{Geometric surface area of catalyst}}$$

The molar flow of Petrol Combusted is obtained assuming the petrol vapour shows ideal gas behaviour, and using the experimental values for the temperature rise across the reactor. The geometric surface area of the catalysts is calculated from the dimensions of the catalyst shown earlier. The example calculation shown below is based on the experimental results obtained on the 12th September 2000 run 1 at an inlet set temperature of 400°C:

1. Mass flowrate of petrol into Reactor

This is calculated from the volumetric flowrate of petrol, and the density of petrol evaluated experimentally as 733 kg/m^3

$$\Rightarrow \quad \text{Mass flowrate of petrol} = \frac{6.1}{60000000} \times 733 = 7.45 \times 10^{-5} \text{ kg/s}$$

2. Molar flowrate of petrol into reactor

This is calculated from the mass flowrate of petrol and the molecular weight of petrol calculated in Chapter 4 as 98 g/mol

$$\Rightarrow \quad \text{Molar flowrate of petrol} = \frac{7.45 \times 10^{-5}}{98} \times 1000 = 7.6 \times 10^{-4} \text{ mol/s}$$

3. Fractional conversion

This is calculated based on the temperature difference between the reactor inlet and reactor outlet after the petrol has been added, and the adiabatic temperature rise expected for 100% conversion of the petrol:

Reactor inlet temperature after the petrol has been added = 387°C
Reactor outlet temperature after the petrol has been added = 465°C

$\Rightarrow$ Temperature rise = 465 – 387 = 78 K

The adiabatic temperature rise for 100% conversion is calculated from an energy balance based on the method already described in Chapter 4 to calculate the fuel flowrate:

$\Rightarrow$ Adiabatic temperature rise for 100% conversion = 300°C

$$\Rightarrow \text{Fractional conversion of petrol} = \frac{78}{300} \times 100 = 26\%$$

4. Molar flowrate of Petrol combusted

This is obtained from the fractional conversion and the molar flowrate of petrol into the reactor:

$\Rightarrow$ Molar flowrate of petrol combusted = $0.26 \times 7.6 \times 10^{-4}$

$= 1.98 \times 10^{-4}$ mol/s

5. Catalyst Geometric surface area.

This was evaluated by the area exposed to reactants through a single channel and then multiplying by the total number of channels in the monoliths

Area for flow through one channel assuming square channels:

= Perimeter of channel exposed to reactants x length of channel

$= (1\times10^{-3}+1\times10^{-3}+1\times10^{-3}+1\times10^{-3}) \times 120\times10^{-3}$

$= 4.8\times10^{-4}$ m^2

Geometric surface area of catalyst = Area of single channel x total number of channels

$= 4.8\times10^{-4} \times 110$

$= 5.25\times10^{-2}$ m^2

6. Observed reaction rate of Petrol across the reactor

This can now be calculated as the molar flowrate of Petrol consumed divided by the total geometric surface area of the catalyst

$$r_{obs} = \frac{1.98x10^{-4}}{5.25x10^{-2}} = 3.76x10^{-3} \text{ mol/s.m}^2$$

This calculation was performed for every inlet set point temperature studied. The results are included with the raw experimental results in Appendix D.

Graphs 5.1 and 5.2, shown at the end of this section, were then plotted of the observed reaction rate against the actual inlet temperature to the reactor for both of the Platinum catalysts investigated.

From these graphs the following conclusions can be drawn:

Platinum Catalyst with 4 g active phase per litre of monolith

1. The observed rate of reaction for the Platinum catalyst with 3wt% active phase is approximately constant over the range of reactor inlet temperatures studied at $5x10^{-3}$ mol/s m^2. This indicates that the rate of reaction is independent of catalyst inlet temperature over the temperature range studied
2. The results are reproducible as both run 1 and run 2 are in good agreement with each other.

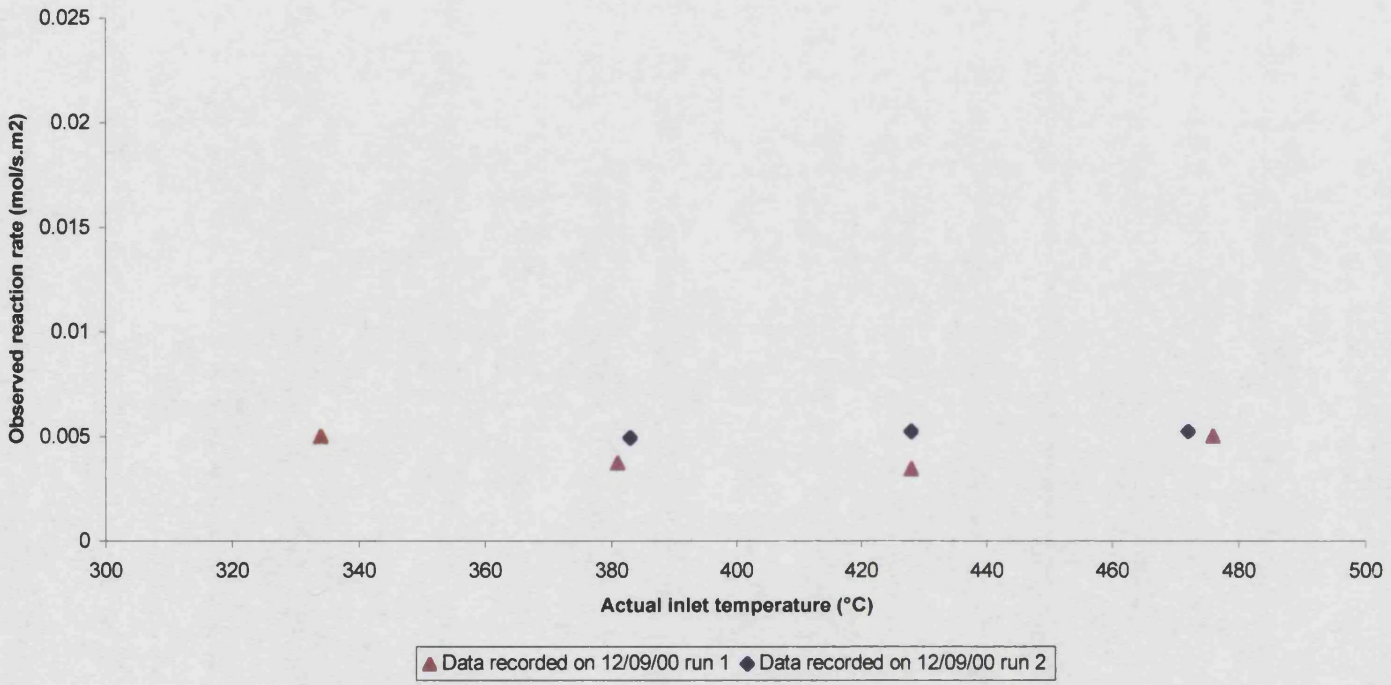
Platinum Catalyst with 8 g active phase per litre of monolith

1. The observed rate of reaction for the Platinum catalyst with 6wt% active phase is approximately constant over the range of reactor inlet temperatures studied at $5x10^{-3}$ mol/s m^2. This indicates that the rate of reaction is independent of catalyst inlet temperature over the temperature range studied.
2. The results are reproducible as both run 1 and run 2 are in good agreement with each other.

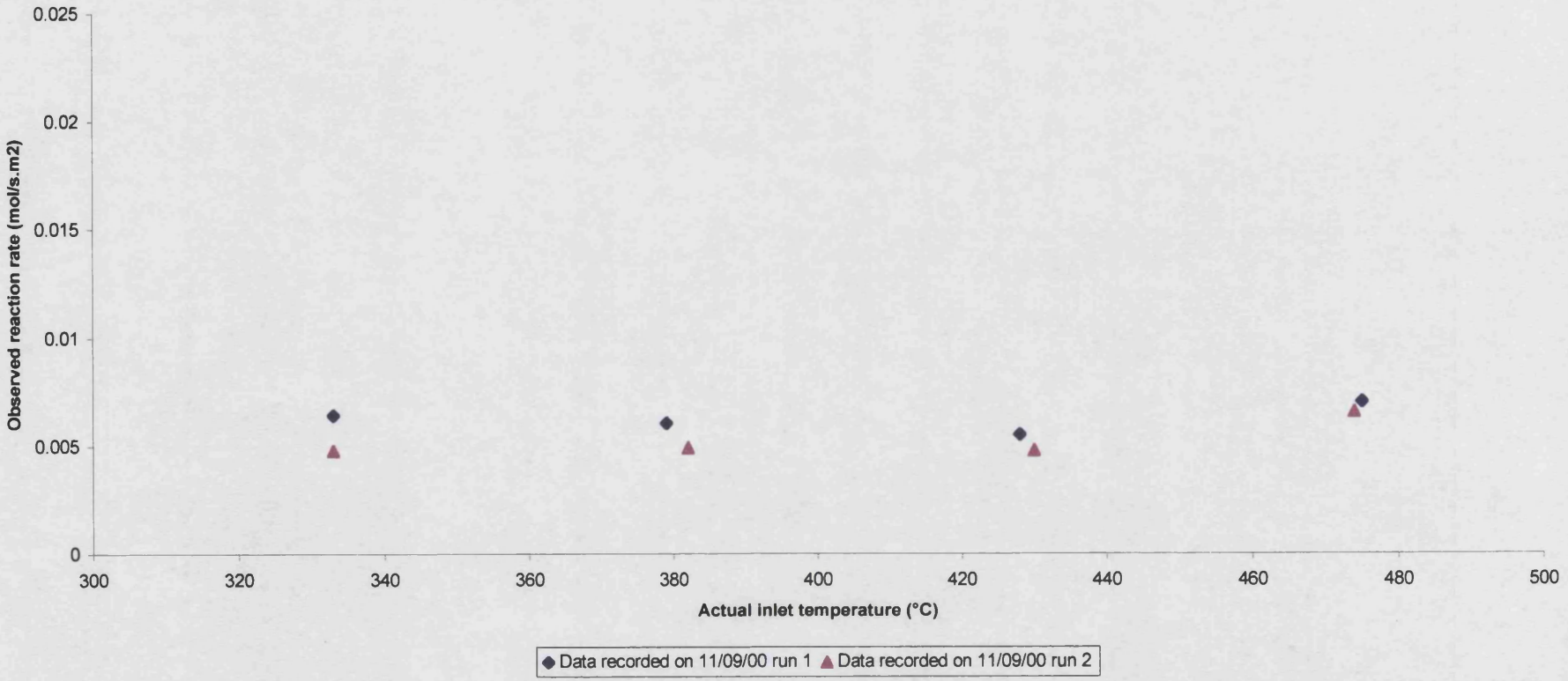
Overall Conclusions

1. The rate of reaction is independent of catalyst inlet temperature for both of the Platinum catalysts, over the range of temperatures studied at $5x10^{-3}$ mol/s m^2
2. Doubling the amount of active phase on the catalyst has had no effect on the rate of reaction observed over the temperature studied.

Graph 5.1: Temperature conversion chart for the catalytic combustion of Unleaded Petrol over Platinum (4g platinum per litre of monolith), at constant pressure of 2 bar gauge, constant mass flow and constant Air:Fuel ratio



Graph 5.2: Temperature conversion chart for the catalytic combustion of Unleaded Petrol over Platinum (8g platinum per litre of monolith), at constant pressure of 2 bar gauge, constant mass flow and constant Air:Fuel ratio



5.1.2 Pressure Effects

In these experiments the effect of changing the reactor pressure on the catalytic combustion of unleaded petrol was investigated. All other conditions in the test rig were fixed. The platinum catalysts were assembled into the test rig as described in Chapter 4. The flowrate of air through the rig was fixed at each different pressure to 500 litres/min (Evaluated at 20°C and 1 bar pressure). The Unleaded Petrol was pumped into the test rig using a metering pump at a fixed rate of 6.1 ml/min, (Chapter 4), (Evaluated at 20°C and 1 bar pressure). The reactor inlet temperature was fixed at 500°C. The pressure in the reactor was varied by adjusting the back-pressure control valve to give pressures varying from 1.5 barg up to 3.5 barg in intervals of 0.5 barg. At each different pressure set point the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in Chapter 3. The experiments were repeated twice and recorded as run 1 and run 2 respectively. The results can be found in Appendix D.

From the raw experimental results, values for the observed reaction rate were calculated as shown previously in the Inlet temperature effects section. These calculated results are included with the raw experimental results in Appendix D.

Values for the Reynolds number through a channel were also calculated from the experimental results as shown below. These results are also included in Appendix D.

The Reynolds number is calculated at the reactor inlet conditions and the Petrol component in the air stream is ignored it is defined as:

$$Re = \frac{\rho U D_e}{\mu}$$

Where:

Re = Reynolds number through a channel

ρ = Density of the air at reactor inlet conditions (kg/m^3)

U = Velocity of air through a channel at inlet conditions (m/s)

D_e = Hydraulic mean diameter (m)

μ = Viscosity of air at reactor inlet conditions (Ns/m^2)

For an example calculation the experimental values obtained during run 1 on 12th September 2000 at a reactor pressure of 2 barg are used:

Inlet temperature after petrol added = 473°C

Pressure of Reactor = 2 barg (3 bar)

1.Volumetric flowrate of Air at reactor inlet temperature and pressure

This is calculated from the Ideal gas law.

$$V_2 = \frac{P_1 V_1 T_2}{T_1 P_2}$$

Where V = Volumetric flowrate (Litres/min)

P = Pressure (Pa)

T = Temperature (K)

Subscripts

1 = Conditions where the volumetric flowrate is known i.e. The flowrate was set to 500 litres/min at 20°C and 1 bar pressure for these experiments.

2 = Conditions where the volumetric flowrate is required i.e. Reactor inlet conditions of 2 barg (3 bar) pressure and actual inlet temperature of 473°C when the petrol was introduced.

$$\Rightarrow \quad V_2 = \frac{1x10^5 * 500 * (473+273)}{(20+273) * 3x10^5} = 424.3 \text{ litre/min} = 7.07x10^{-3} \text{m}^3/\text{s}$$

2. Molar flowrate of Air

This is calculated from the volumetric flowrate of air, and assuming that the air behaves as an ideal gas, such that the ideal gas law can be used:

From $PV = mRT \quad \Rightarrow \quad m = \frac{PV}{RT}$

Where m = Molar flowrate (mol/s)

P = Reactor inlet Pressure = 2 barg (3 bar)

V = Volumetric flowrate of air into reactor = $7.07x10^{-3}$ m^3/s

T = Reactor inlet temp = 473°C (Inlet temp after Petrol added)

R = Universal gas Constant = 8.314 J/mol K

$\Rightarrow \quad m = 0.34$ mol/s

3. Mass flowrate of air

This can be obtained from:

Mass flowrate of air = Molar flowrate of air * Molar mass of air

$= 0.34*29 = 9.86$ g/s $= 9.9x10^{-3}$ kg/s

4. Density of air

This is obtained as:

$$\Rightarrow \rho = \frac{\text{Mass flowrate air}}{\text{Volumetric flowrate of air}} = \frac{9.9x10^{-3}}{7.07x10^{-3}} = 1.4 \text{kg/m}^3$$

5. Velocity of air through a channel

This is calculated by:

$$\text{Velocity through a Channel} = \frac{\text{Volumetric flowrate of air}}{\text{Number of Channels} * \text{Area of a channel}}$$

$$= \frac{7.07x10^{-3}}{110*1x10^{-3}*1x10^{-3}} = 64.5\text{m/s}$$

6. Hydraulic mean diameter of a channel

This is defined as:

$$D_e = \frac{4*\text{Surface area for flow}}{\text{Wetted perimeter}}$$

The Surface area for flow = $1x10^{-3} * 1x10^{-3}$ (square channels) = $1x10^{-6}m^2$

The Wetted Perimeter = Perimeter of the channel

$$= (1x10^{-3}+1x10^{-3}+1x10^{-3}+1x10^{-3})$$

$$= 4x10^{-3}\text{ m}$$

$\Rightarrow$ $D_e = 1x10^{-3}$ m

7. Viscosity of air at inlet temperature and pressure

This was calculated using predictive methods as described in the literature [Perry 1984]:

$\mu = 3.55x10^{-5}$ Ns/m^2

8. Reynolds number through a channel

As defined earlier the Reynolds number through a channel is:

$$\mathrm{Re} = \frac{\rho U D_e}{\mu}$$

$\Rightarrow$ Re obtained for the sample calculation conditions = 2549

Having calculated the observed reaction rate and Reynolds number through a channel for each pressure studied the following graphs were plotted:

1. *Graphs 5.3 and 5.4* The temperature rise across the catalysts against reactor pressure for both Platinum catalysts (4 g/l and 8 g/l).
2. *Graphs 5.5 and 5.6* The Observed reaction rate against reactor pressure for both Platinum catalysts (4 g/l and 8 g/l).
3. *Graphs 5.7 and 5.8* The Reynolds number through a channel against reactor
   pressure for both Platinum catalysts (4 g/l and 8 g/l).

These graphs are all shown in at the end of this section.

From these graphs the following conclusions can be drawn:

Platinum Catalyst with 4 g active phase per litre of monolith

1. As the pressure is increased from 1.5 barg to 3.5 barg the temperature rise across the reactor increases from approx a 95°C rise to a 160°C rise at 3.5 barg. This indicates that more of the Petrol present in the air is being combusted at the higher pressures.
2. The observed reaction rate also increases with pressure. At 1.5 barg the reaction rate is approx $4.5x10^{-3}$ mol/s m^2. This rises to a value of $7.5x10^{-3}$ mol/s m^2 at 3.5 barg. This shows that the rate of reaction of Petrol is affected by pressure. The higher values of pressure give a larger reaction rate hence more petrol is combusted.
3. The Reynolds number through a channel remains approximately constant with pressure at 2550. This indicates Transitional flow through the channels, and that the observed increase in reaction rate noticed with increasing pressure is not a result of changes in the Reynolds number.
4. All the results are repeatable as both run 1 and run 2 are in close agreement.

Platinum Catalysts with 8 g active phase per litre of monolith

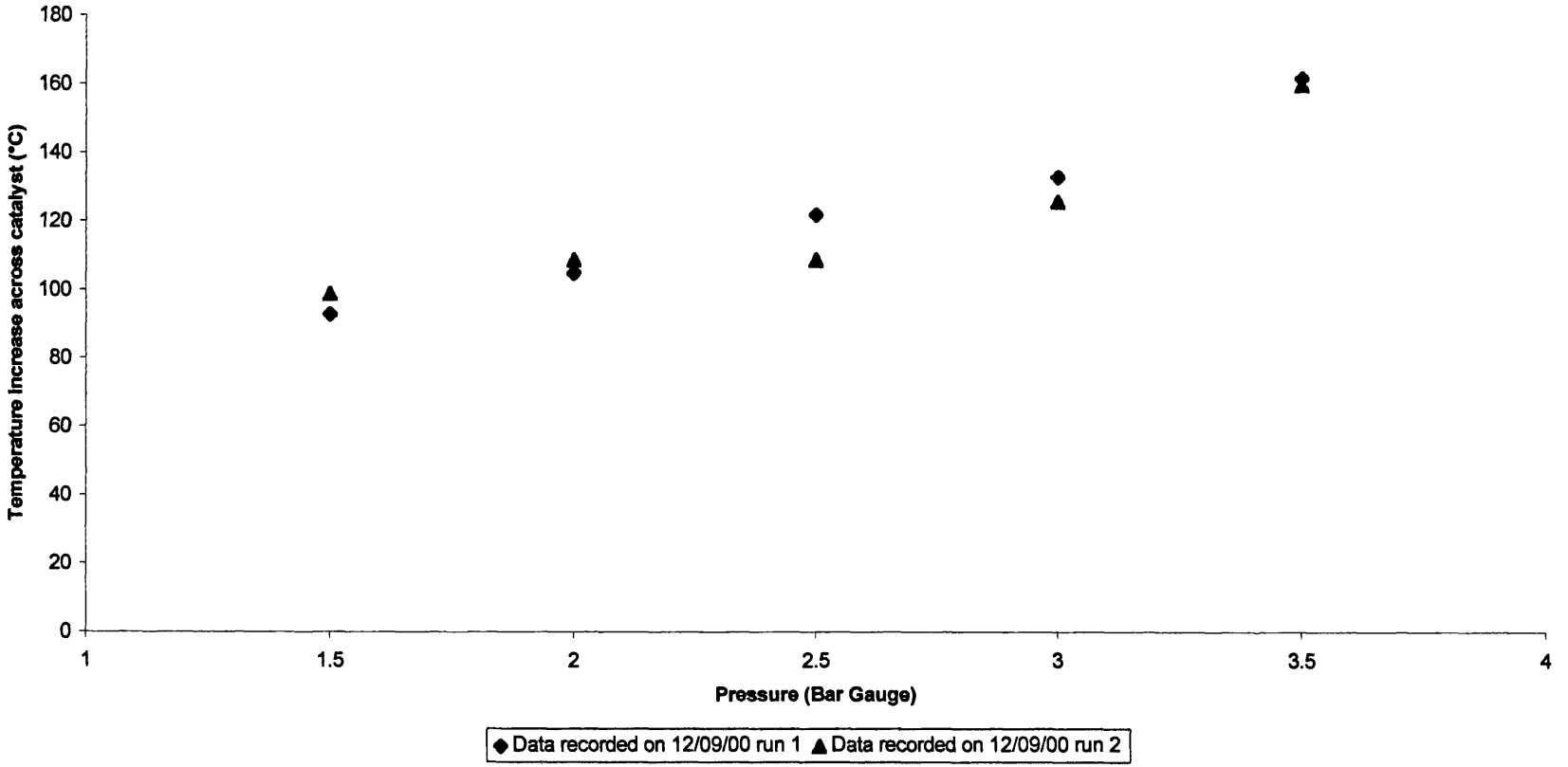
1. As the pressure is increased from 1.5 barg to 3.5 barg the temperature rise across the reactor increases from approx a 140°C to a 200°C rise at 3.5 barg. This indicates that more of the Petrol present in the air is being combusted at the higher pressures.
2. The observed reaction rate increases slightly with pressure. At 1.5 barg the observed reaction rate is approx $6.5x10^{-3}$ mol/s m^2, and rises to a value of approx $9.0x10^{-3}$ mol/s m^2 at 3.5 barg. This shows that the rate of reaction of Petrol is slightly affected by pressure. The higher values of pressure give a larger reaction rate hence more petrol is combusted.

3. The Reynolds number through a channel shows minor fluctuations with pressure, but is approx constant at 2550 over the range of pressures studied. This indicates Transitional flow through the channels, and that the observed changes in the rate of reaction noticed with increasing pressure is not a result of changes in the Reynolds number.
4. All the results are repeatable as both run 1 and run 2 are in close agreement.

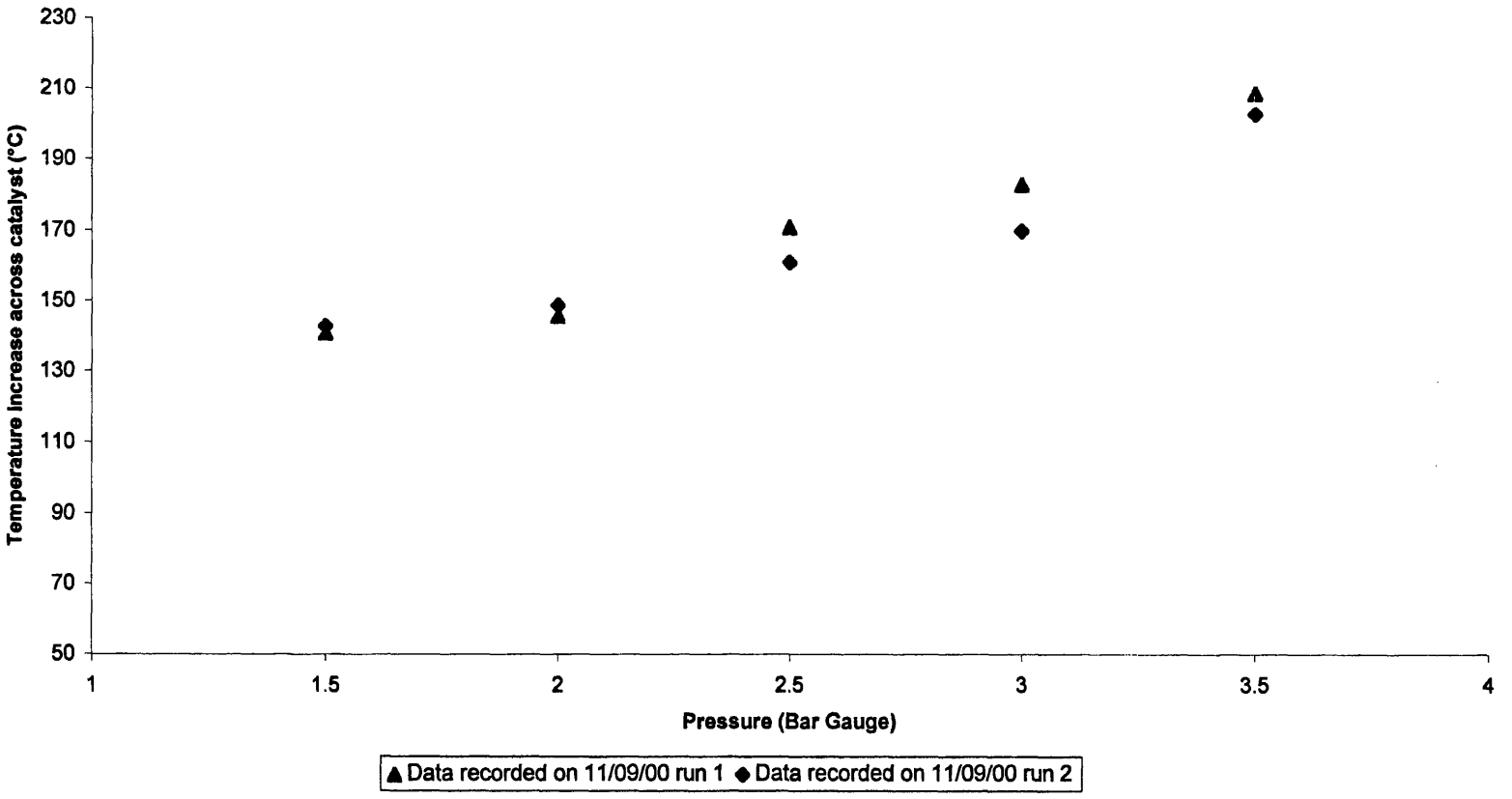
Overall conclusions

1. The Observed rate of reaction is dependent on the reactor pressure. Higher pressures show an increase in the observed rate of reaction, which is also shown by an increase in the temperature rise across the catalyst bed.
2. Both the platinum catalysts show this trend.
3. Doubling the amount of platinum active phase on the catalysts shows an increase in the observed rate of reaction over the pressure range studied. At 1.5 barg the 8 g/l platinum catalyst shows an increase in the observed rate of reaction by a factor of 1.44, compared to the catalyst with 4 g/l platinum. At 3.5 barg the 8 g/l platinum catalyst shows an increase in the observed rate of reaction by a factor of 1.20, compared to the catalyst with 4 g/l.
4. The Reynolds numbers through a channel remain unchanged with reactor pressure, and are similar for both the platinum catalysts at approx 2550. The flow through the channels is in the transitional regime for both the catalysts.

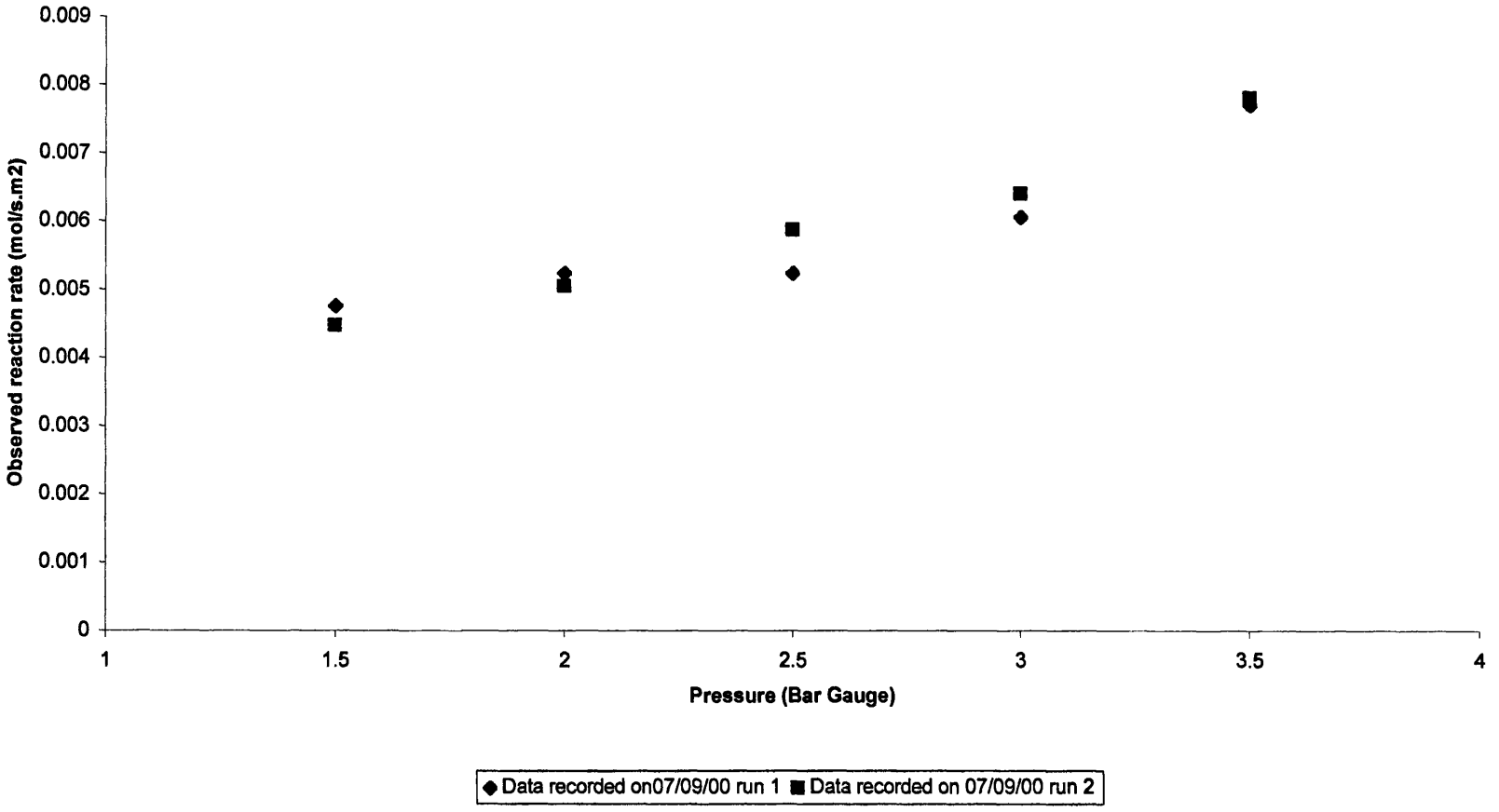
Graph 5.3: Effect of pressure on the catalytic combustion of Unleaded Petrol over Platinum (4g platinum per litre of monolith), at a constant throughput and a constant inlet setpoint temperature of 500°C



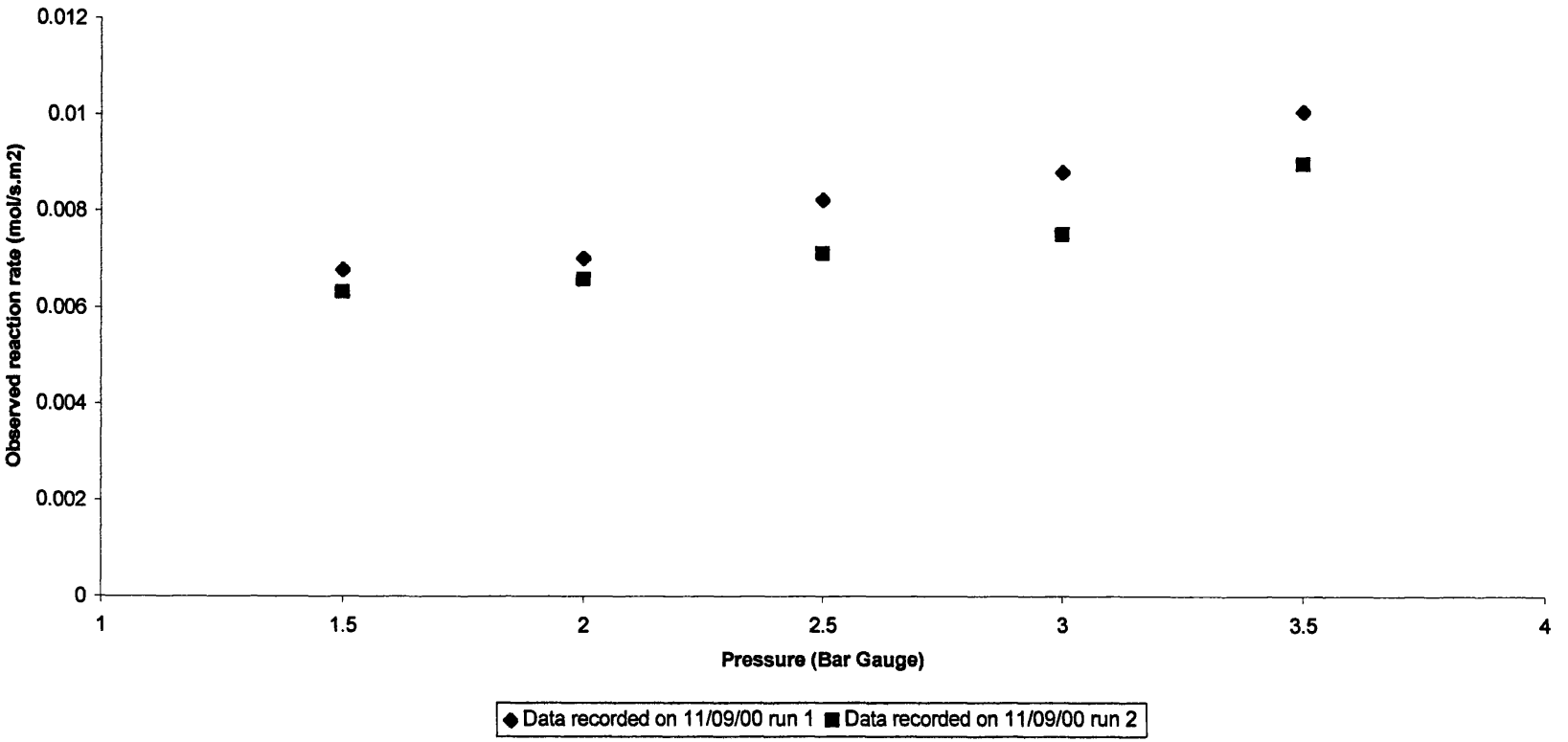
Graph 5.4: Effect of pressure on the catalytic combustion of Unleaded Petrol over Platinum (8g platinum per litre of monolith), at a constant throughput and a constant inlet setpoint temperature of 500°C



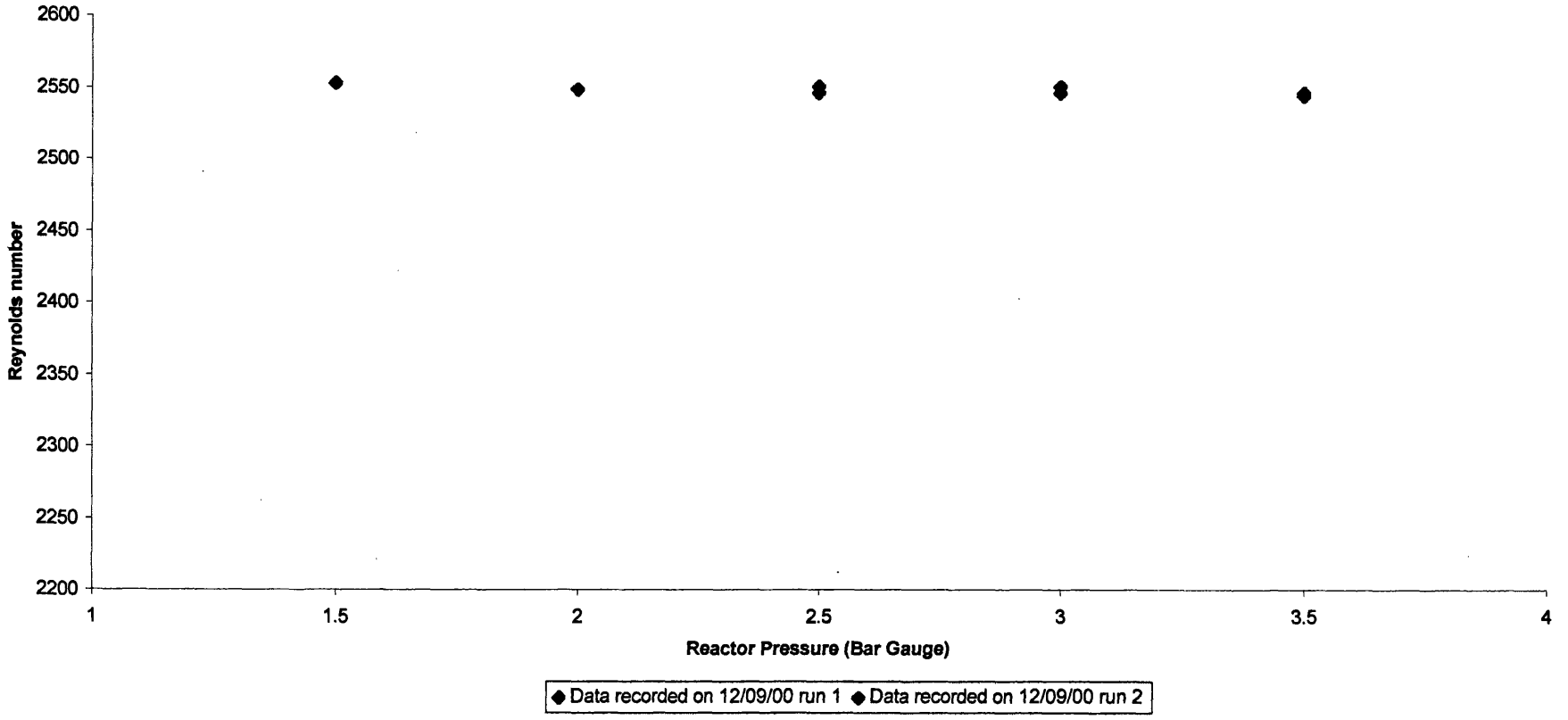
Graph 5.5: Effect of pressure on the catalytic combustion of Unleaded Petrol over Platinum (4g platinum per litre of monolith), at a constant throughput and a constant inlet setpoint temperature of 500°C



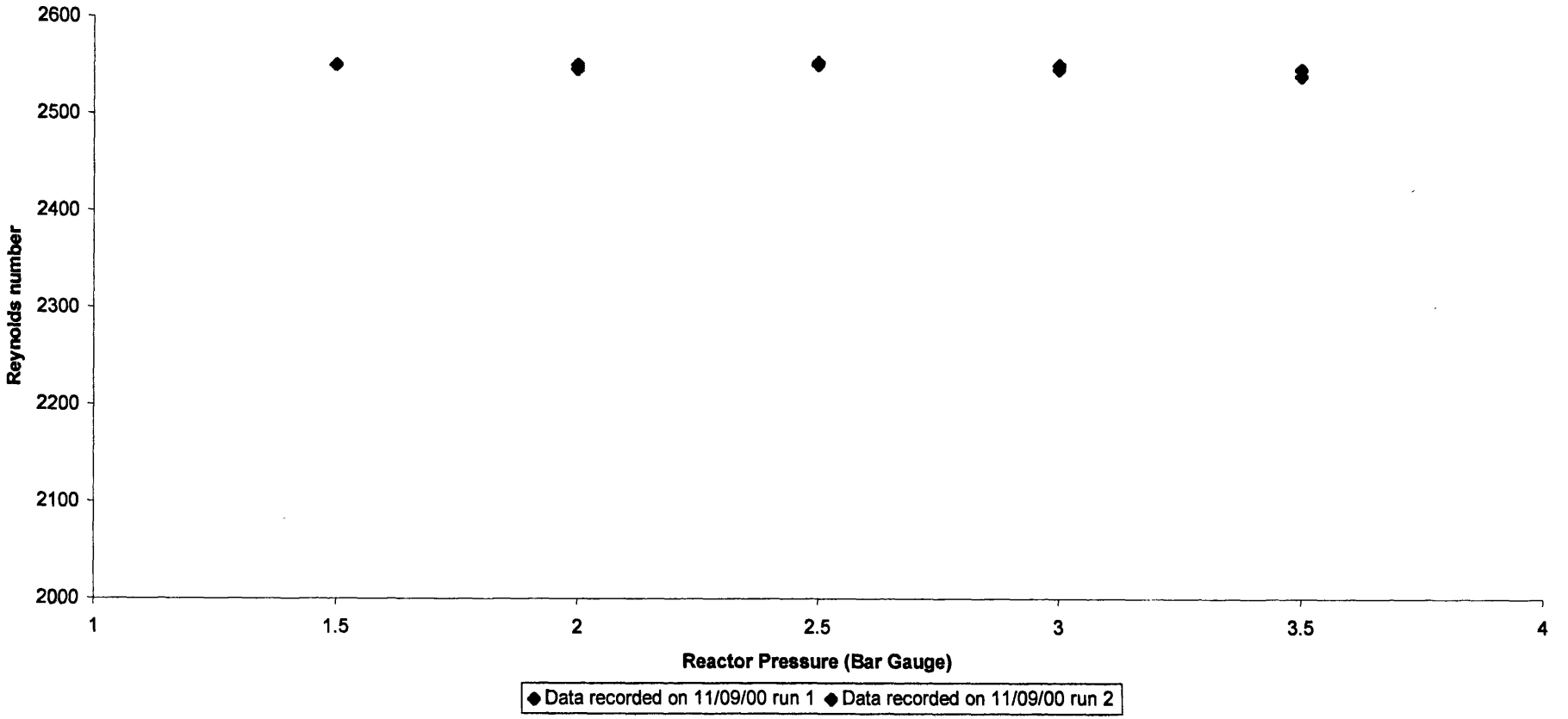
Graph 5.6: Effect of pressure on the catalytic combustion of Unleaded Petrol over Platinum (8g platinum per litre of monolith), at a constant throughput and a constant inlet setpoint temperature of 500°C



Graph 5.7: Reynolds number against reactor pressure for the catalytic combustion of Unleaded Petrol over Platinum (4g platinum per litre of monolith), at constant throughput and constant inlet setpoint temperature of 500°C



Graph 5.8: Reynolds number against reactor pressure for the catalytic combustion of Unleaded Petrol over Platinum (8g platinum per litre of monolith), at constant throughput and constant inlet setpoint temperature of 500°C



5.1.3 Fuel flowrate effects

In these experiments the effect of changing the fuel flowrate on the catalytic combustion of unleaded petrol was investigated. All other conditions in the test rig were fixed. Only the 4 g platinum per litre of monolith catalyst was used for these experiments and the catalyst was assembled into the test rig as described in Chapter 4. The flowrate of air through the rig was fixed for each fuel flowrate to 500 litres/min (Evaluated at 20°C and 1 bar pressure). The Unleaded Petrol was pumped into the test rig using a metering pump and varied. The range of fuel flowrates studied was 3, 4.6, 6.1 and 7.6 ml/min (Evaluated at 20°C and 1 bar pressure). The reactor inlet temperature was fixed at 500°C, and the pressure in the reactor was maintained constant at 2.0 barg. For each different fuel flowrate the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in Chapter 3. The results can be found in Appendix D.

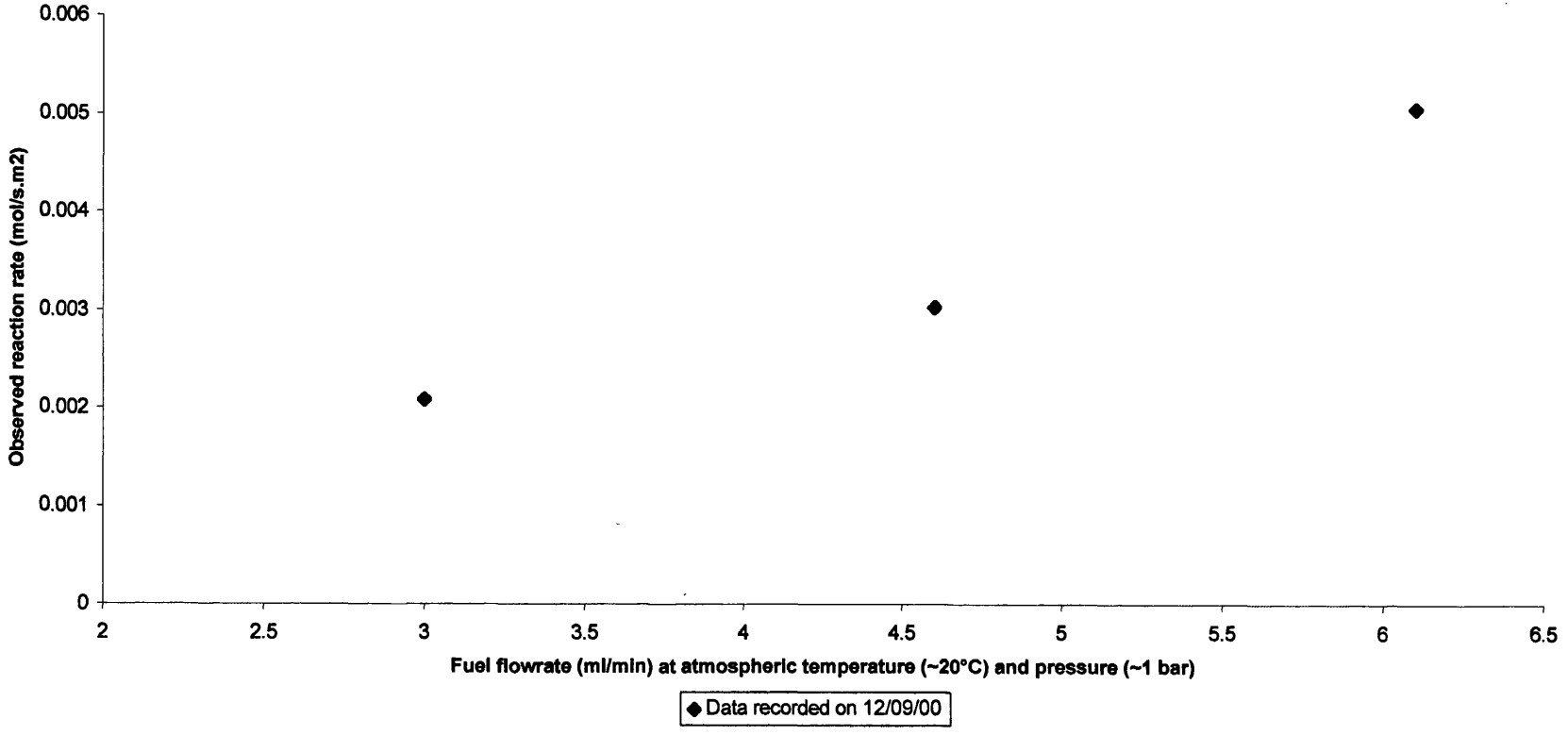
From the raw experimental results, values for the observed reaction rate were calculated as shown previously in the Inlet temperature effects section. The adiabatic temperature rise for 100% conversion was recalculated as necessary for the different fuel flowrates used.
These calculated results are included with the raw experimental results in Appendix D.

Graph 5.9 was then plotted showing the observed reaction rate against the fuel flowrate and is included at the end of this section.

From the graph the following conclusions can be drawn:

1. The observed rate of reaction increased with an increase in the petrol flowrate. At petrol flowrate of 3 ml/min the observed reaction rate was $2.0x10^{-3}$ mol/s m^2, and increased to a value of approx $5.0x10^{-3}$ mol/s m^2 at a petrol flowrate of 7.6 ml/min.
2. The catalytic combustion of petrol is dependent on the petrol flowrate. At low petrol flowrates less of the available petrol is combusted than at high petrol flowrates, where more of the available petrol is combusted

Graph 5.9: Effect of changing Fuel flowrate on the catalytic combustion of Unleaded Petrol over Platinum catalyst (4g platinum per litre of monolith) at constant pressure of 2 bar gauge, constant air flowrate of 500 l/min and constant inlet temp of 500°C



5.1.4 Total mass flowrate effects.

In these experiments the effect of changing the total mass flowrate on the catalytic combustion of unleaded petrol was investigated. All other conditions in the test rig were fixed. Only the 4 g platinum per litre of monolith catalyst was used for these experiments and the catalyst was assembled into the test rig as described in Chapter 4. The flowrate of air through the rig was varied along with the petrol flowrate such that at each total flowrate studied the air to fuel ratio (by mol) remained constant at 457.4. The ranges of air and petrol flowrates studied are shown in the following table. All flowrates were recorded at atmospheric temperature and pressure (20°C and 1 bar.)

Air flowrate (l/min)	Petrol flowrate (ml/min)	Air to Fuel ratio (mol basis)	Equivalence Ratio
250	3.0	457.4	0.0152
500	6.0	457.4	0.0152
750	9.0	457.4	0.0152

Experiments were performed at fixed pressures of 2.0 barg and then repeated at 3.5 barg. The reactor inlet set temperature was fixed at 400°C, and the experiments were then repeated for inlet set temperatures of 450°C and 500°C, at both the fixed pressures of 2.0 barg and 3.5 barg. For each different total flowrate the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in Chapter 3. The results can be found in Appendix D.

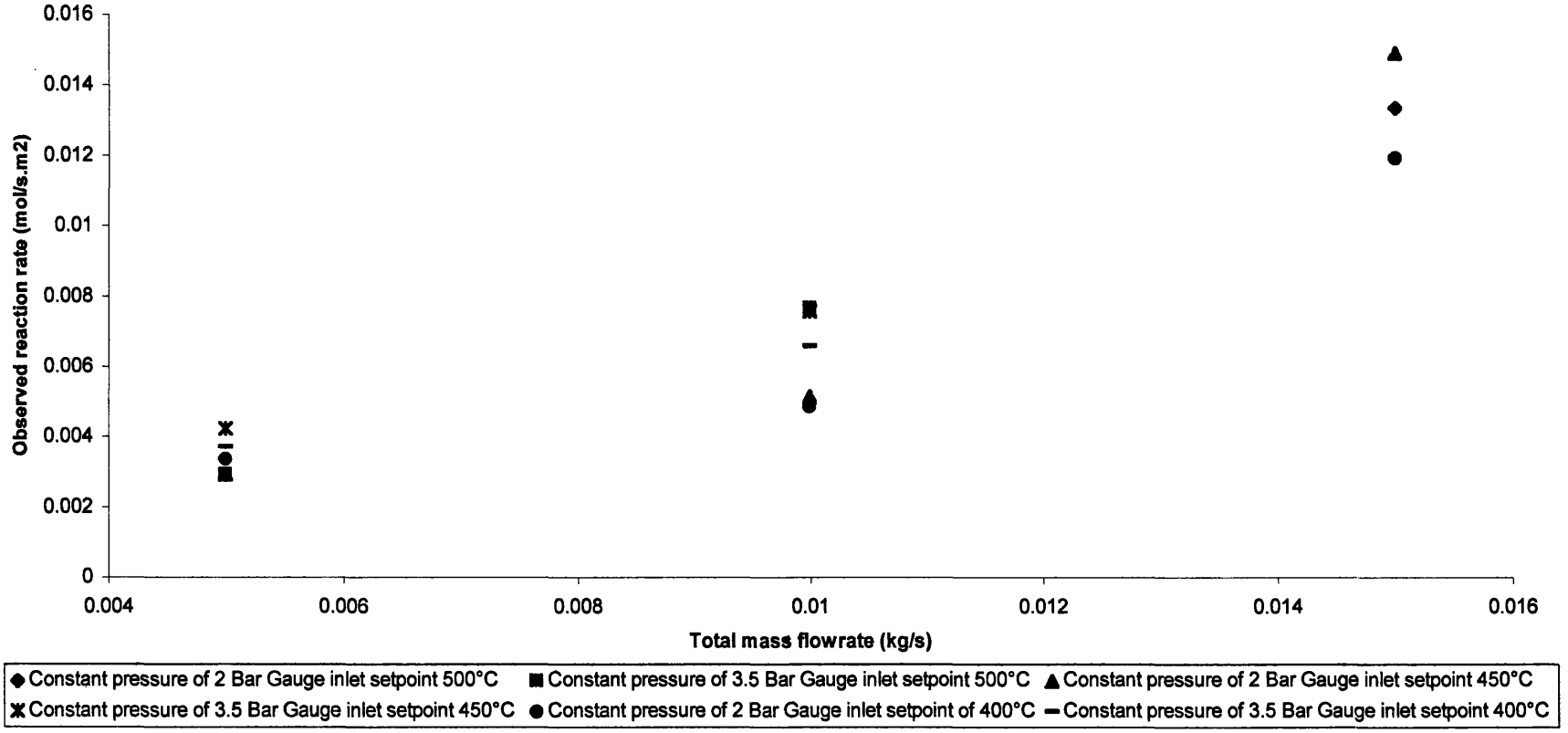
From the raw experimental results, values for the observed reaction rate were then calculated as shown previously in the Inlet temperature effects section. These calculated results are included with the raw experimental results in Appendix D.

A graph of the observed reaction rate against the total mass flowrate for both set pressures and inlet temperatures was then plotted (*Graph 5.10*), and is shown at then end of this section.

From the graph the following conclusions can be drawn:

1. The observed rate of reaction increases with an increase in the total mass flowrate. This indicates that the catalytic combustion is mass transfer limited even through the flowrate is transitional through a channel.
2. The trend is repeated for both pressures, and all of the inlet temperatures studied.
3. At the largest total mass flowrate studied (0.015 kg/s), the observed reaction rate is highest for a reactor pressure of 2 barg and inlet temperature set point of 450°C (0.015 mol/s m^2), and is lowest for a reactor pressure of 2 barg and inlet set point of 400°C (0.013 mol/s m^2).
4. At the lowest total mass flowrate studied (0.005 kg/s), the observed reaction rates are all similar with an approx value of 0.003 mol/s m^2.

Graph 5.10: Effect of total mass flowrate on the catalytic combustion of Unleaded Petrol over Platinum (4g platinum per litre of monolith), at constant Air:Fuel ratio. Date recorded on 12th Sept 2000



5.2 Results for the Catalytic Combustion of Unleaded Petrol over $LaMnO_3$ Perovskite type Catalysts.

Experiments were performed using $LaMnO_3$ perovskite type catalysts of fixed dimensions. All monoliths had an initial gamma alumina washcoat layer of approx 112 g alumina per litre of monolith, which were calcinated to 500°C. The Perovskite active phase of $LaMnO_3$ was added to give finial catalysts with approx 24 g $LaMnO_3$ per litre of monolith. The finished catalysts were calcinated to 800°C. Full details on the production of the catalysts can be found in Chapter 4.

5.2.1 Inlet Temperature effects.

In these experiments the effect of changing the catalyst inlet temperature on the catalytic combustion of unleaded petrol was investigated. All other conditions in the test rig were fixed. The perovskite catalysts were assembled into the test rig as described in Chapter 4. The flowrate of air through the rig was fixed at 500 litres/min (Evaluated at 20°C and 1 bar pressure). The Unleaded Petrol was pumped into the test rig using a metering pump at a fixed rate of 6.1 ml/min, (Chapter 4), (Evaluated at 20°C and 1 bar pressure). The reactor pressure was fixed at 2 barg using a back-pressure control valve. The catalyst inlet temperature was varied by altering the electric air heater set point from 350°C to 500°C in increments of 50°C. At each different temperature set point the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in Chapter 3. The experiment was repeated twice recorded as run 1 and run 2 respectively. The results can be found in Appendix E.

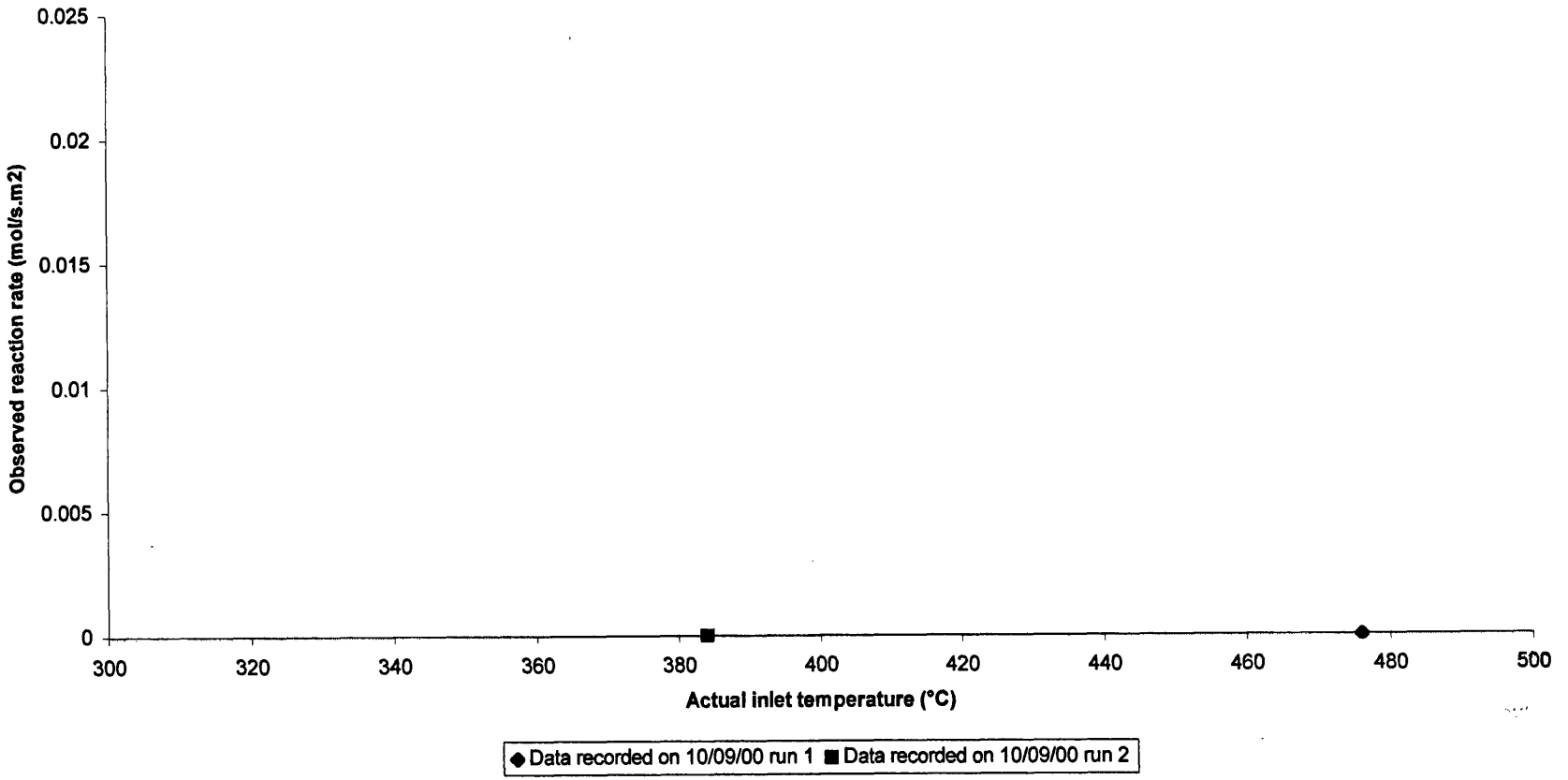
From the raw experimental results, values for the observed reaction rate were calculated as shown described in the inlet temperature effects for platinum catalysts section.

A graph was then plotted of the observed reaction rate against the actual inlet temperature to reactor for the perovskite catalyst (*Graph 5.11*). This is shown at the end of this section.

From the graph the following conclusions can be drawn:

1. The perovskite catalyst shows no activity for the combustion of unleaded petrol, over the inlet temperature range studied. This is indicated by the observed rate of reaction being approx 0 for all the inlet temperatures studied.
2. The results are repeatable as the values of the observed rate of reaction for run 1 and run 2 are in good agreement.

Graph 5.11: Temperature conversion chart for the catalytic combustion of Unleaded Petrol over $LaMnO_3$ perovskite, (24g $LaMnO_3$ per litre of monolith), at constant pressure of 2 bar gauge, constant mass flow and constant Air:Fuel ratio



5.3 Results for the Catalytic Combustion of Unleaded Petrol over an industrial Catalyst supplied by Degussa.

Experiments were performed using an industrial catalyst supplied by Degussa. The active phase was disclosed as being platinum with a loading of approx 4 g platinum per litre of monolith. Full details on the Degussa catalyst can be found in Chapter 4.

5.3.1 Inlet Temperature effects.

In these experiments the effect of changing the catalyst inlet temperature on the catalytic combustion of unleaded petrol was investigated. All other conditions in the test rig were fixed. The Degussa catalyst was assembled into the test rig as described in Chapter 4. The flowrate of air through the rig was fixed at 500 litres/min (Evaluated at 20°C and 1 bar pressure). The Unleaded Petrol was pumped into the test rig using a metering pump at a fixed rate of 6.1 ml/min, (Chapter 4), (Evaluated at 20°C and 1 bar pressure). The reactor pressure was fixed at 2 barg using a back-pressure control valve. The catalyst inlet temperature was varied by altering the electric air heater set point from 350°C to 500°C in increments of 50°C. At each different temperature set point the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in Chapter 3. The experiment was repeated twice recorded as run 1 and run 2 respectively. The results can be found in Appendix F.

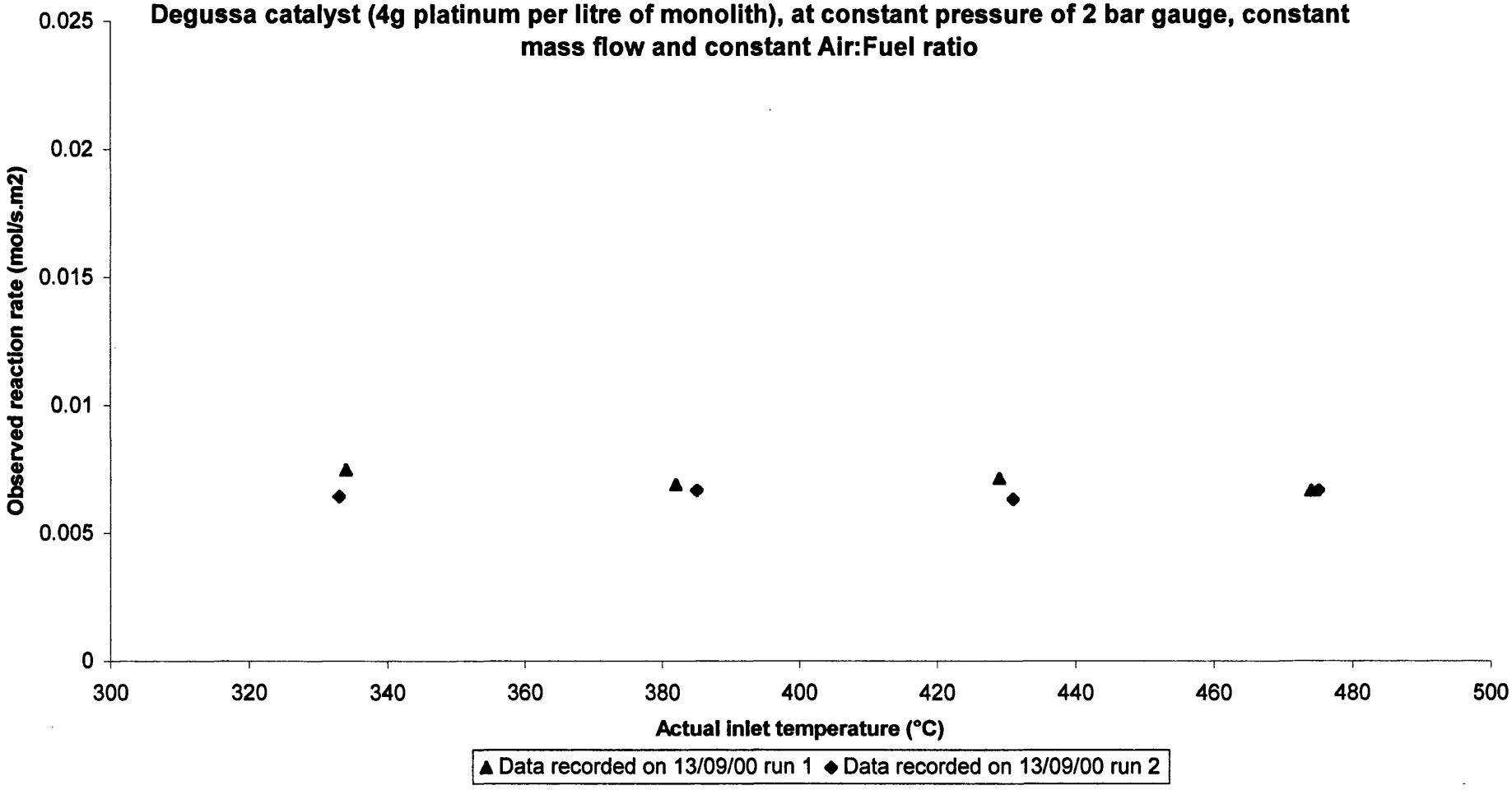
From the raw experimental results, values for the observed reaction rate were calculated as previously described in the inlet temperature effects for platinum catalysts section.

A graph was then plotted of the observed reaction rate against the actual inlet temperature to reactor for the Degussa catalyst (*Graph 5.12*). This is shown at the end of this section.

From the graph the following conclusions can be drawn:

1. The observed rate of reaction for the Degussa catalyst with 3 wt% active phase is approximately constant over the range of reactor inlet temperatures studied at $7x10^{-3}$ mol/s m^2. This indicates that the rate of reaction is independent of catalyst inlet temperature over the temperature range studied
2. The results are reproducible as both run 1 and run 2 are in good agreement with each other.

Graph 5.12: Temperature conversion chart for the catalytic combustion of Unleaded Petrol over Degussa catalyst (4g platinum per litre of monolith), at constant pressure of 2 bar gauge, constant mass flow and constant Air:Fuel ratio



5.3.2 Pressure Effects

In these experiments the effect of changing the reactor pressure on the catalytic combustion of unleaded petrol was investigated. All other conditions in the test rig were fixed. The Degussa catalysts were assembled into the test rig as described in Chapter 4. The flowrate of air through the rig was fixed at each different pressure to 500 litres/min (Evaluated at 20°C and 1 bar pressure). The Unleaded Petrol was pumped into the test rig using a metering pump at a fixed rate of 6.1 ml/min, (Chapter 4), (Evaluated at 20°C and 1 bar pressure). The reactor inlet temperature was fixed at 500°C. The pressure in the reactor was varied by adjusting the back-pressure control valve to give pressures varying from 1.5 barg up to 3.5 barg in intervals of 0.5 barg. At each different pressure set point the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in Chapter 3. The experiments were repeated twice and recorded as run 1 and run 2 respectively. The results can be found in Appendix F.

From the raw experimental results, values for the observed reaction rate could be calculated as shown previously. Values for the Reynolds number through a channel were also calculated. These results are included with the raw experimental results in Appendix F.

Having calculated the observed reaction rate and Reynolds number through a channel for each pressure studied the following graphs were plotted:

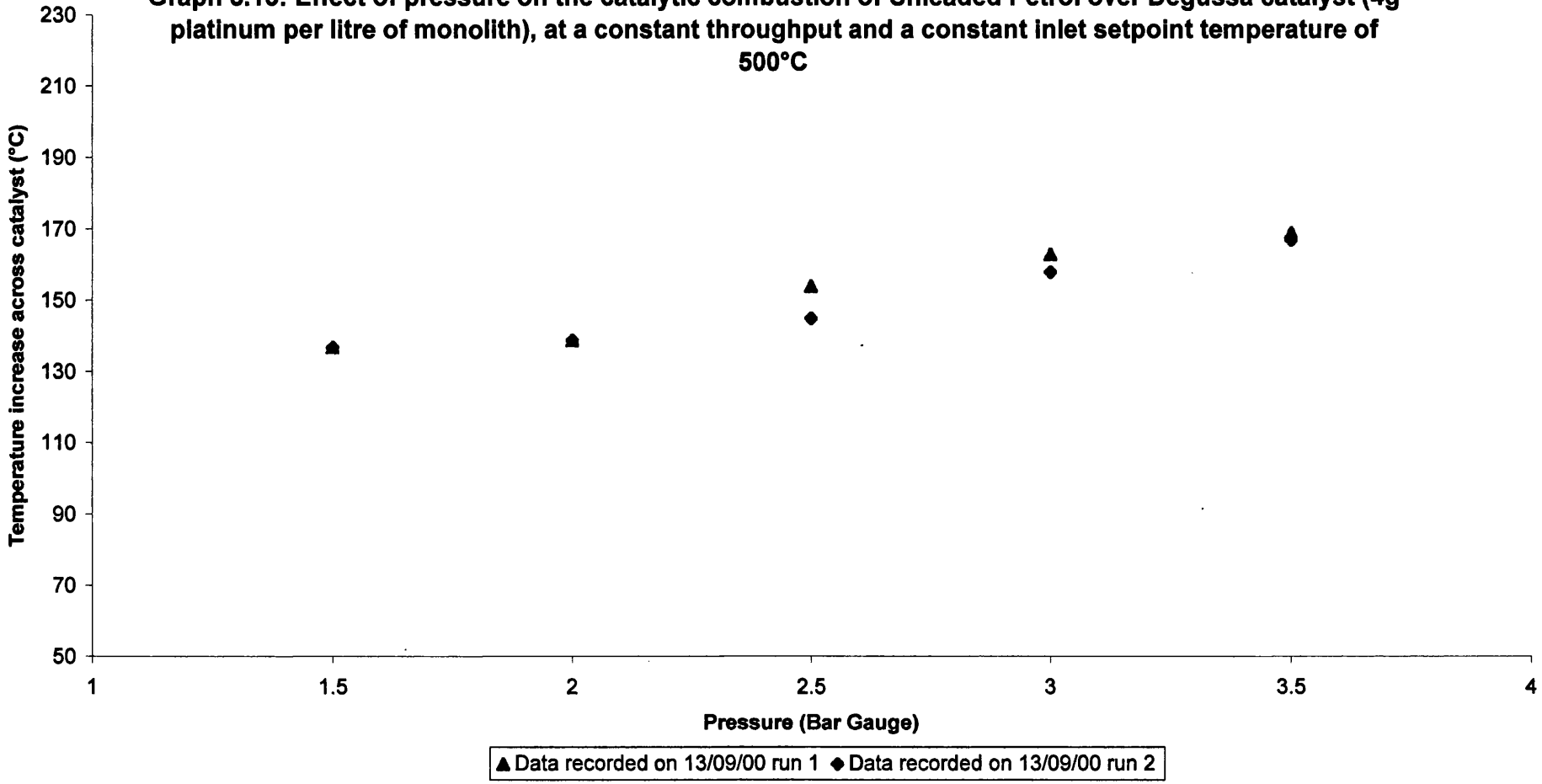
1. The temperature rise across the catalysts against reactor pressure (*Graph 5.13*).
2. The Observed reaction rate against reactor pressure (*Graph 5.14*).
3. The Reynolds number through a channel against reactor pressure (*Graph 5.15*).

These graphs are all shown at the end of this section.

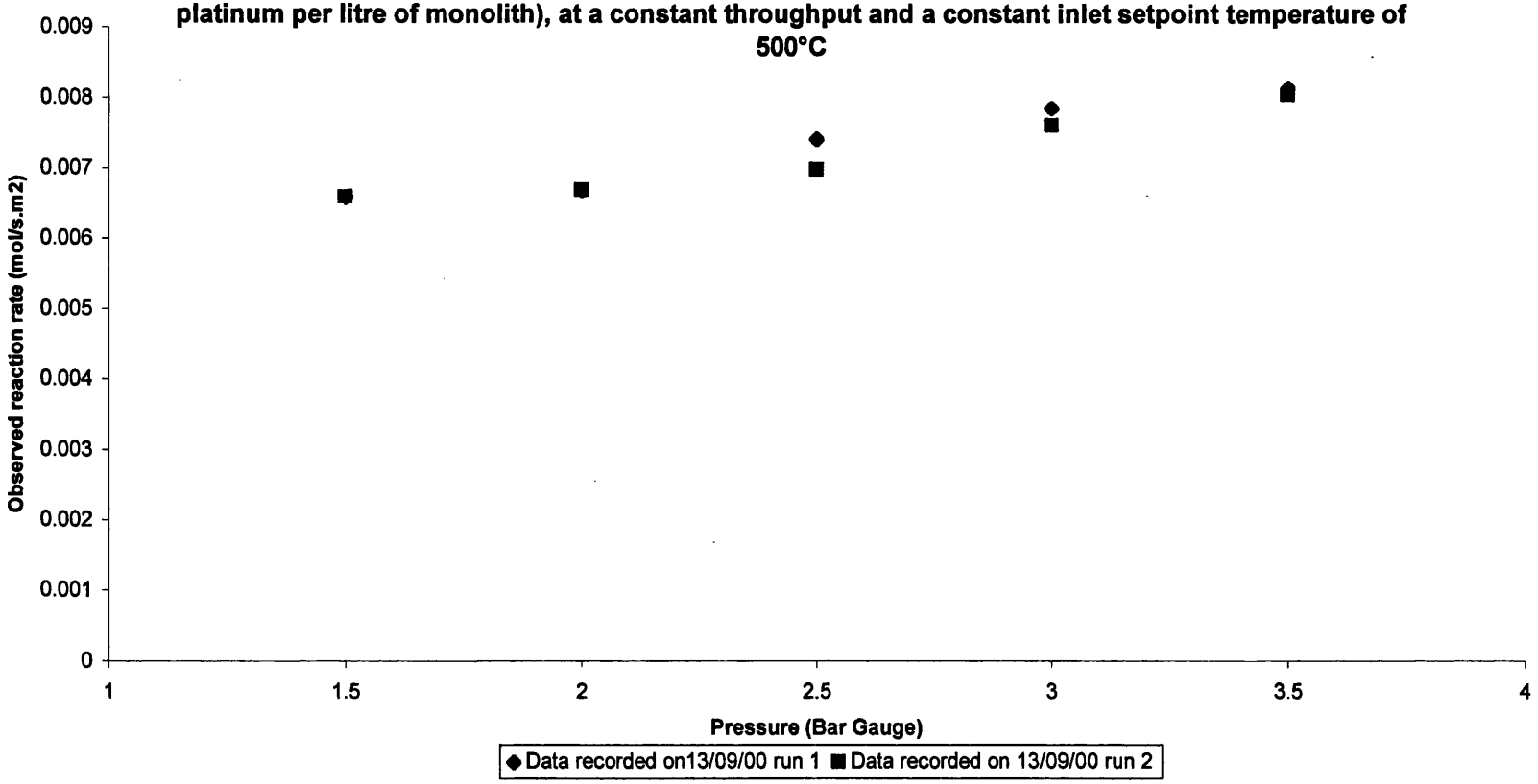
From these graphs the following conclusions can be drawn:

1. The temperature increase across the catalyst increases slightly with pressure. At 1.5 barg the temperature change is approx 135 K, while at 3.5 barg the temperature increase across the catalyst is approx 160 K. This indicates that the catalytic combustion of unleaded petrol using the Degussa catalyst shows a slight dependence on pressure.
2. The observed rate of reaction increases slightly with an increase in pressure. At 1.5 barg the observed rate of reaction is approx $6.5x10^{-3}$ mol/s m^2, which increases to approx $8.0x10^{-3}$ mol/s m^2 at 3.5 barg. The increase indicates that the catalytic combustion of unleaded petrol over the Degussa catalysts is only slightly dependent on pressure.
3. The Reynolds number through a channel shows minor fluctuations with pressure, but is approx constant at 2550 over the range of pressures studied. This indicates Transitional flow through the channels, and that the observed changes in the rate of reaction noticed with increasing pressure is not a result of changes in the Reynolds number.
4. All the results are repeatable as both run 1 and run 2 are in close agreement.

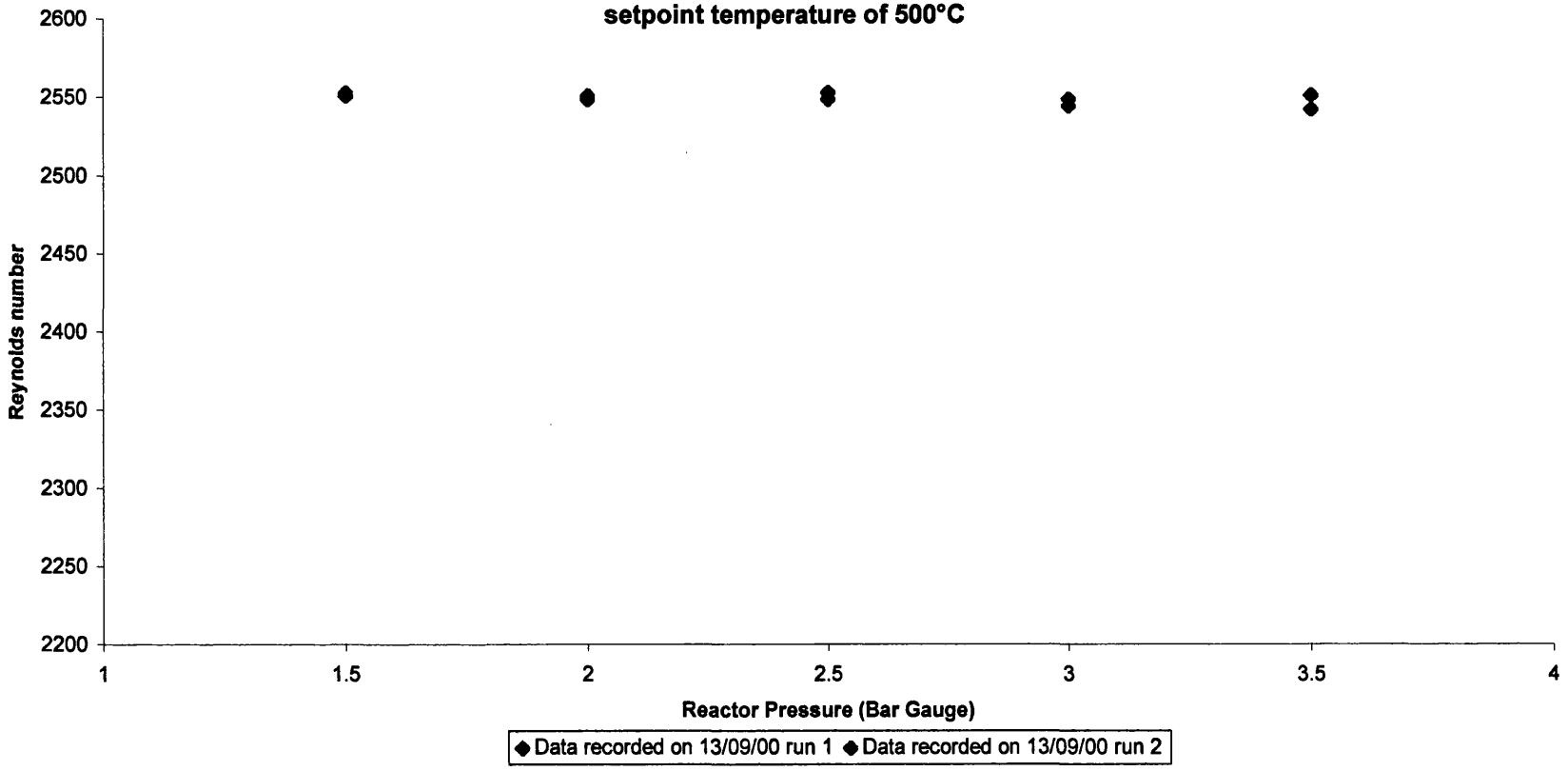
Graph 5.13: Effect of pressure on the catalytic combustion of Unleaded Petrol over Degussa catalyst (4g platinum per litre of monolith), at a constant throughput and a constant inlet setpoint temperature of 500°C



Graph 5.14: Effect of pressure on the catalytic combustion of Unleaded Petrol over Deguusa catalyst (4g platinum per litre of monolith), at a constant throughput and a constant inlet setpoint temperature of 500°C



Graph 5.15: Reynolds number against reactor pressure for the catalytic combustion of Unleaded Petrol over Degussa catalyst (4g platinum per litre of monolith), at constant throughput and constant inlet setpoint temperature of 500°C



Chapter 6: Results for the Catalytic Combustion of Diesel Fuel.

6.1 Results obtained using Platinum Catalysts.

Experiments were performed using platinum catalysts of fixed dimensions, with two different amounts of active phase. All monoliths had an initial gamma alumina washcoat layer of approx 112 g alumina per litre of monolith, which were calcinated to 500°C. The Platinum active phase was added to give final catalysts with approx 4 g Platinum per litre of monolith, and 8 g Platinum per litre of monolith. Both finished catalysts were calcinated to 800°C. Full details on the production of the catalysts can be found in the Chapter 4.

6.1.1 Inlet Temperature effects.

In these experiments the effect of changing the catalyst inlet temperature on the catalytic combustion of Diesel fuel was investigated. All other conditions in the test rig were fixed. The platinum catalysts were assembled into the test rig as described in the Chapter 3. The flowrate of air through the rig was fixed at 500 litres/min (Evaluated at 20°C and 1 bar pressure). The Diesel Fuel was pumped into the test rig using a metering pump at a fixed rate of 5.6 ml/min, (Chapter 4), (Evaluated at 20°C and 1 bar pressure). The reactor pressure was fixed at 2 barg using a back-pressure control valve. The catalyst inlet temperature was varied by altering the electric air heater set point from 350°C to 500°C in increments of 50°C. At each different temperature set point the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in the Chapter 3. The experiment was repeated twice recorded as run 1 and run 2 respectively. The results can be found in Appendix G.

From the raw experimental results, values for the observed reaction rate were calculated as shown previously in Chapter 5. The calculation was performed for every inlet set point temperature studied, and the results are included with the raw experimental results in Appendix G.

Graphs were then plotted of the observed reaction rate against the actual inlet temperature to the reactor for both of the Platinum catalysts investigated (*Graphs 6.1 and 6.2*). These are shown at the end of this section.

From these graphs the following conclusions can be drawn:

Platinum Catalyst with 4 g active phase per litre of monolith

1. The observed rate of reaction for the Platinum catalyst with 4 g active phase per litre of monolith is approximately constant over the range of reactor inlet temperatures studied at 3.3×10^{-3} mol/s m^2. This indicates that the rate of reaction is independent of catalyst inlet temperature over the temperature range studied.
2. The results are reproducible as both run 1 and run 2 are in good agreement with each other.

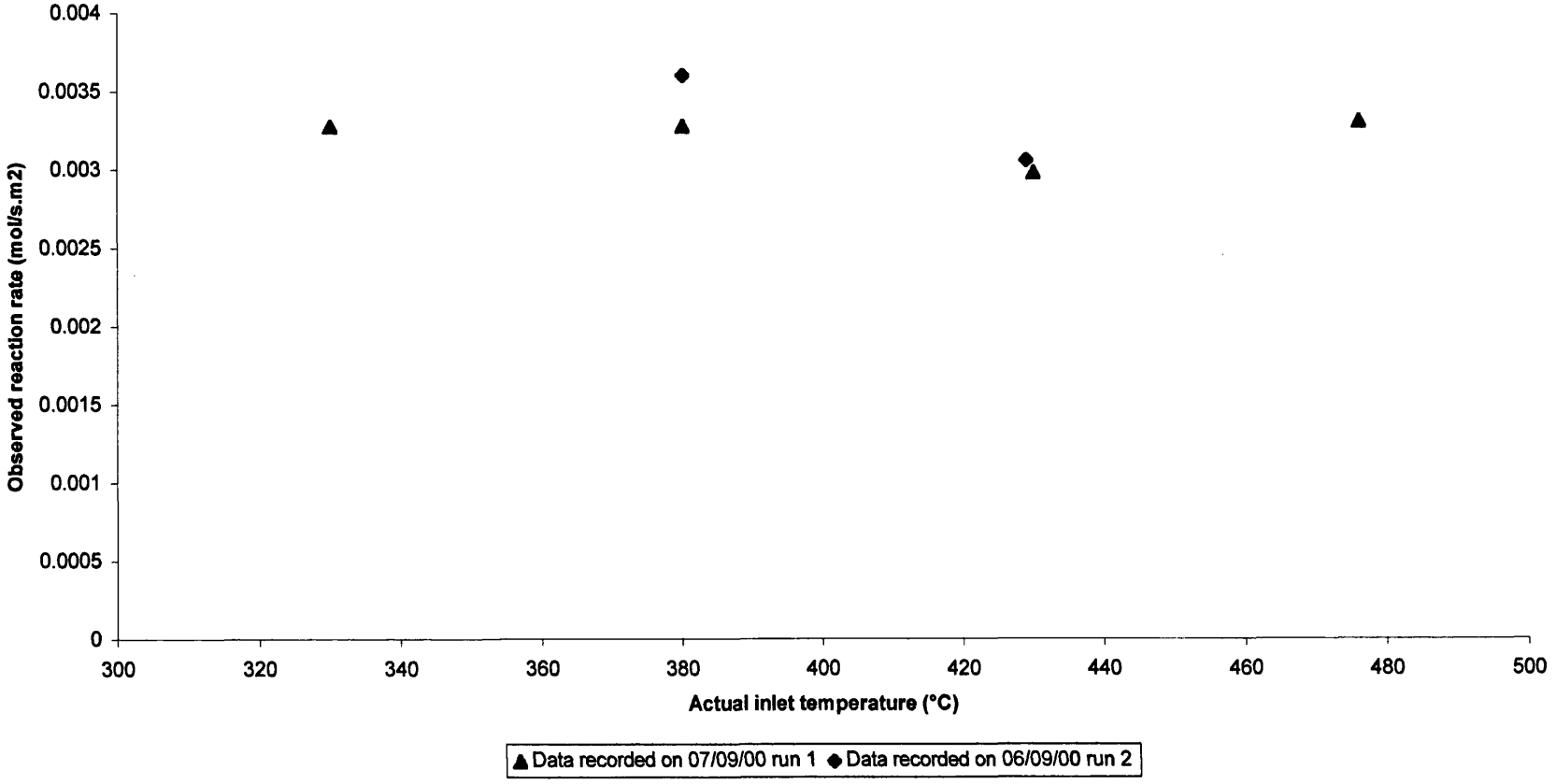
Platinum Catalyst with 8 g active phase per litre of monolith

1. The observed rate of reaction for the Platinum catalyst with 8 g active phase per litre of monolith is approximately constant over the range of reactor inlet temperatures studied at 4.0×10^{-3} mol/s m^2. This indicates that the rate of reaction is independent of catalyst inlet temperature over the temperature range studied.
2. The results are reproducible as both run 1 and run 2 are in good agreement with each other.

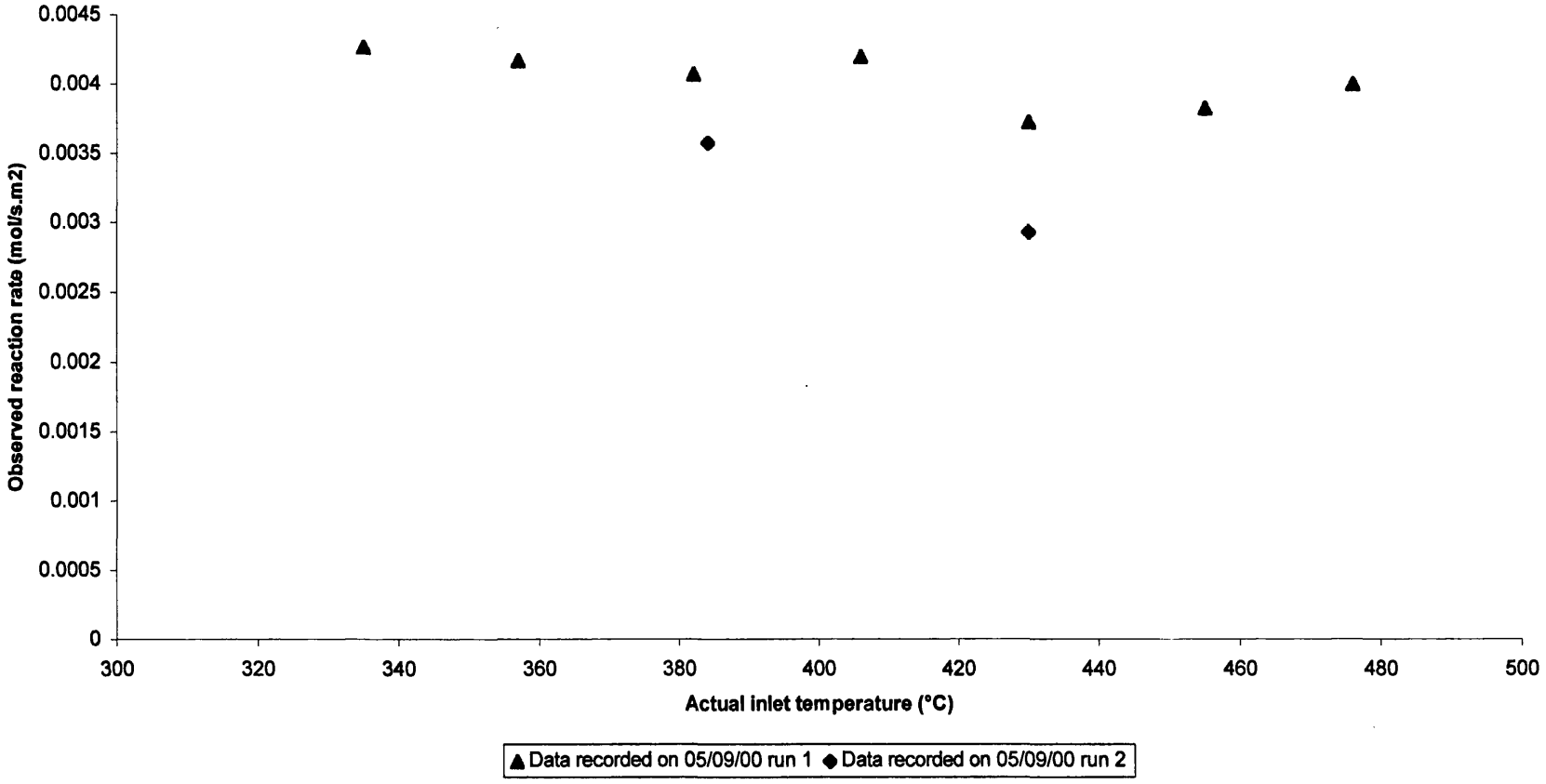
Overall Conclusions

1. The rate of reaction is independent of catalyst inlet temperature for both of the Platinum catalysts, over the range of temperatures studied at $3.3x10^{-3}$ mol/s m^2 for the catalyst with 4 g Platinum per litre of monolith and 4.0 $x10^{-3}$ mol/s m^2 for the catalyst with 8 g Platinum per litre of monolith.
2. Doubling the amount of platinum active phase on the catalyst has increased the observed rate of reaction by a factor of approx 1.21

Graph 6.1: Temperature conversion chart for the catalytic combustion of Diesel fuel over Platinum (4g Active phase per litre of monolith), at constant pressure of 2 bar gauge, constant mass flow and constant Air:Fuel ratio



Graph 6.2: Temperature conversion chart for the catalytic combustion of Diesel fuel over Platinum (8g Active phase per litre of monolith), at constant pressure of 2 bar gauge, constant mass flow and constant Air:Fuel ratio



6.1.2 Pressure Effects

In these experiments the effect of changing the reactor pressure on the catalytic combustion of Diesel fuel was investigated. All other conditions in the test rig were fixed. The platinum catalysts were assembled into the test rig as described in the Chapter 4. The flowrate of air through the rig was fixed at each different pressure to 500 litres/min (Evaluated at 20°C and 1 bar pressure). The Diesel fuel was pumped into the test rig using a metering pump at a fixed rate of 5.6 ml/min, (Chapter 4), (Evaluated at 20°C and 1 bar pressure). The reactor inlet temperature was fixed at 500°C. The pressure in the reactor was varied by adjusting the back-pressure control valve to give pressures varying from 1.5 barg up to 3.5 barg in intervals of 0.5 barg. At each different pressure set point the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in the Chapter 3. The experiments were repeated twice and recorded as run 1 and run 2 respectively. The results can be found in Appendix G.

From the raw experimental results, values for the observed reaction rate were calculated as shown previously in Chapter 5. These calculated results are included with the raw experimental results in Appendix G.

Values for the Reynolds number through a channel were also calculated from the experimental results as described in Chapter 5. These results are also included in Appendix G.

Having calculated the observed reaction rate and Reynolds number through a channel for each pressure studied the following graphs were plotted:

1. The temperature rise across the catalysts against reactor pressure for both Platinum catalysts (*Graphs 6.3 and 6.4*).
2. The Observed reaction rate against reactor pressure for both Platinum catalysts (*Graphs 6.5 and 6.6*).
3. The Reynolds number through a channel against reactor pressure for both Platinum catalysts (*Graphs 6.7 and 6.8*).

These graphs are all shown at the end of this section.

From these graphs the following conclusions can be drawn:

Platinum Catalyst with 4 g active phase per litre of monolith

1. As the pressure is increased from 1.5 barg to 2 barg the temperature rise across the reactor remains constant at 130°C. From 2 barg to 2.5 barg the temperature increase across the reactor increases sharply to 175°C. The temperature increase then says constant at 175°C for the remaining pressures.
2. The observed reaction rate increases with pressure. At 1.5 barg the reaction rate is approx 3.5×10^{-3} mol/s m^2. This rises to a value of 4.7×10^{-3} mol/s.m^2 at 3.5 barg. This shows that the rate of reaction of Diesel fuel is affected by pressure. The higher values of pressure give a larger observed reaction rate hence more of the available Diesel fuel is combusted.
3. The Reynolds number through a channel remains approximately constant with pressure at 2500. This indicates Transitional flow through the channels, and that the observed increase in reaction rate noticed with increasing pressure is not a result of changes in the Reynolds number.
4. All the results are repeatable as both run 1 and run 2 are in close agreement.

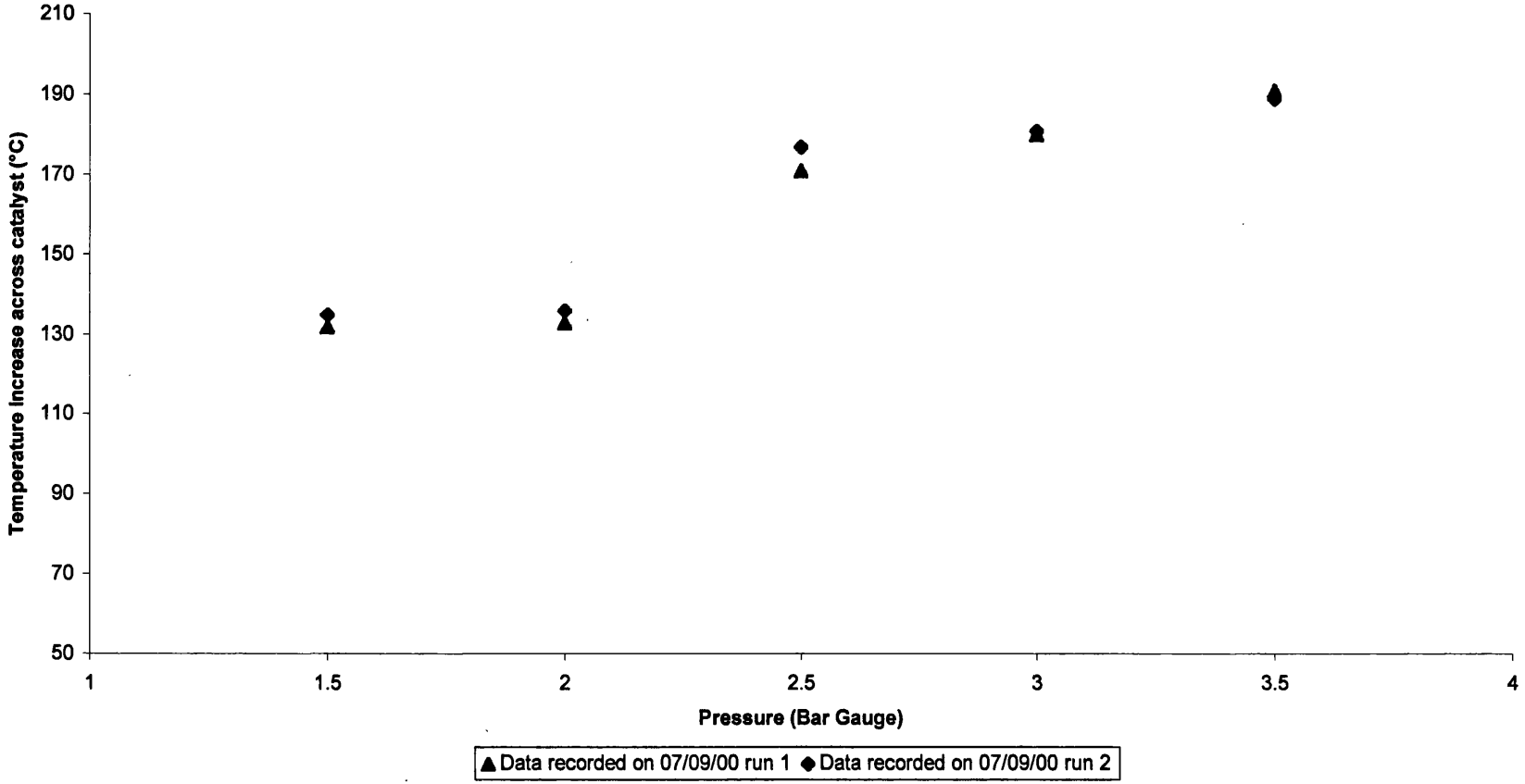
Platinum Catalysts with 8 g active phase per litre of monolith.

1. As the pressure is increased from 1.5 barg to 3.5 barg the temperature rise across the reactor increases slightly from approx a 150°C to a 200°C rise at 3.5 barg. This indicates that more of the Diesel fuel present in the air is being combusted at the higher pressures.
2. The observed reaction rate also changes slightly with pressure. At 1.5 barg the observed reaction rate is approx $3.5x10^{-3}$ mol/s m^2. The observed reaction rate then increases with pressure to a value of approx $5.0x10^{-3}$ mol/s m^2 at 3.5 barg
3. The Reynolds number through a channel shows minor fluctuations with pressure, but is approx constant at 2500 over the range of pressures studied. This indicates Transitional flow through the channels, and that the observed changes in the rate of reaction noticed with increasing pressure is not a result of changes in the Reynolds number.
4. All the results are repeatable as both run 1 and run 2 are in close agreement.

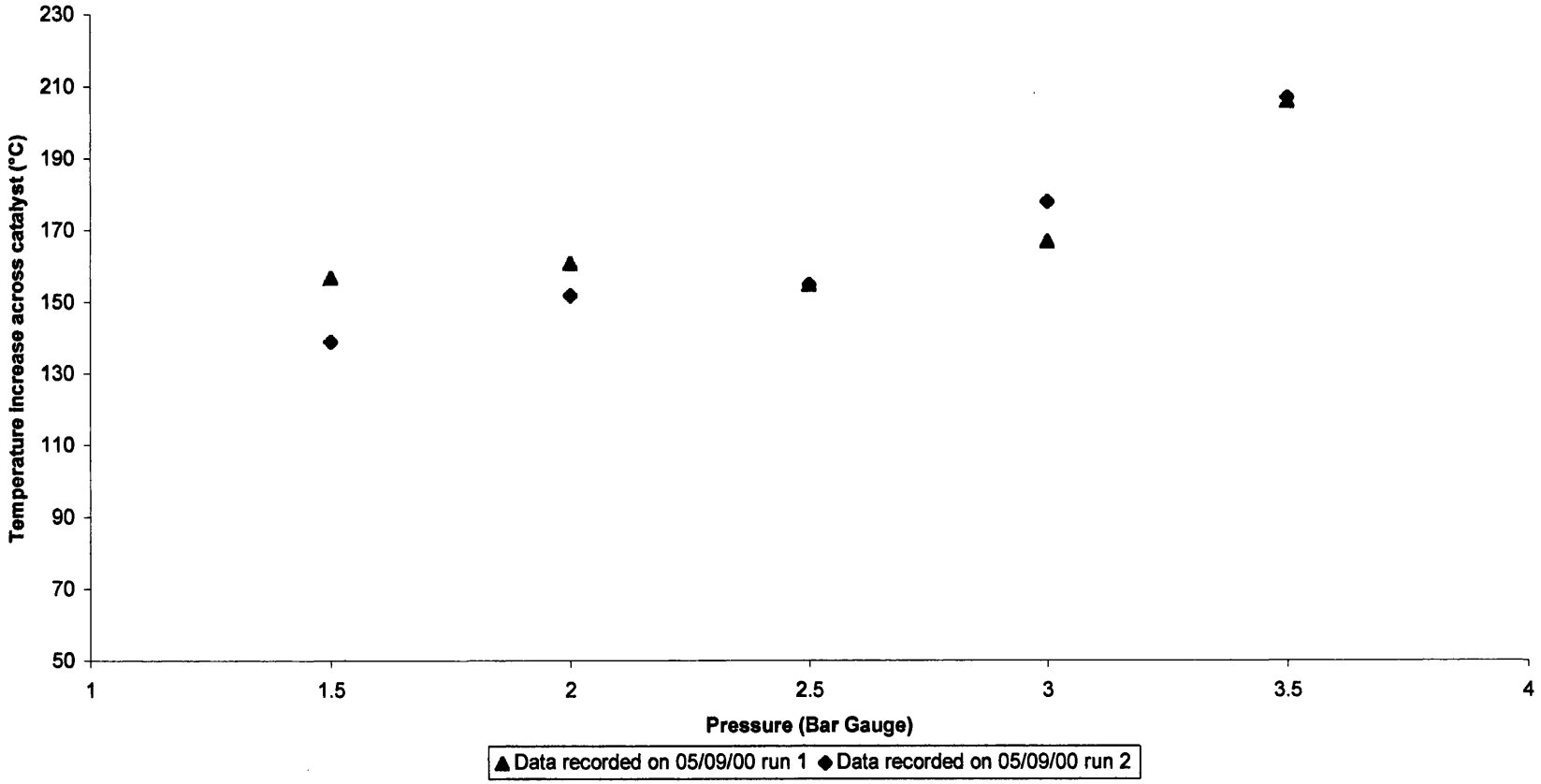
Overall conclusions

1. The Observed rate of reaction is dependent on the reactor pressure. Higher pressures show an increase in the observed rate of reaction, which is also shown by an increase in the temperature rise across the catalyst bed.
2. This trend is more pronounced by the platinum catalyst with 4 g active phase per litre of monolith.
3. Doubling the amount of platinum active phase on the catalyst increases the temperature rise across the reactor from 130°C to 150°C at 1.5 barg and from 175°C to 200°C at 3.5 barg.
4. Doubling the amount of platinum active phase on the catalyst has little affect on the observed rate of reaction.
5. The Reynolds numbers through a channel remain unchanged with reactor pressure, and are similar for both the platinum catalysts at approx 2500.

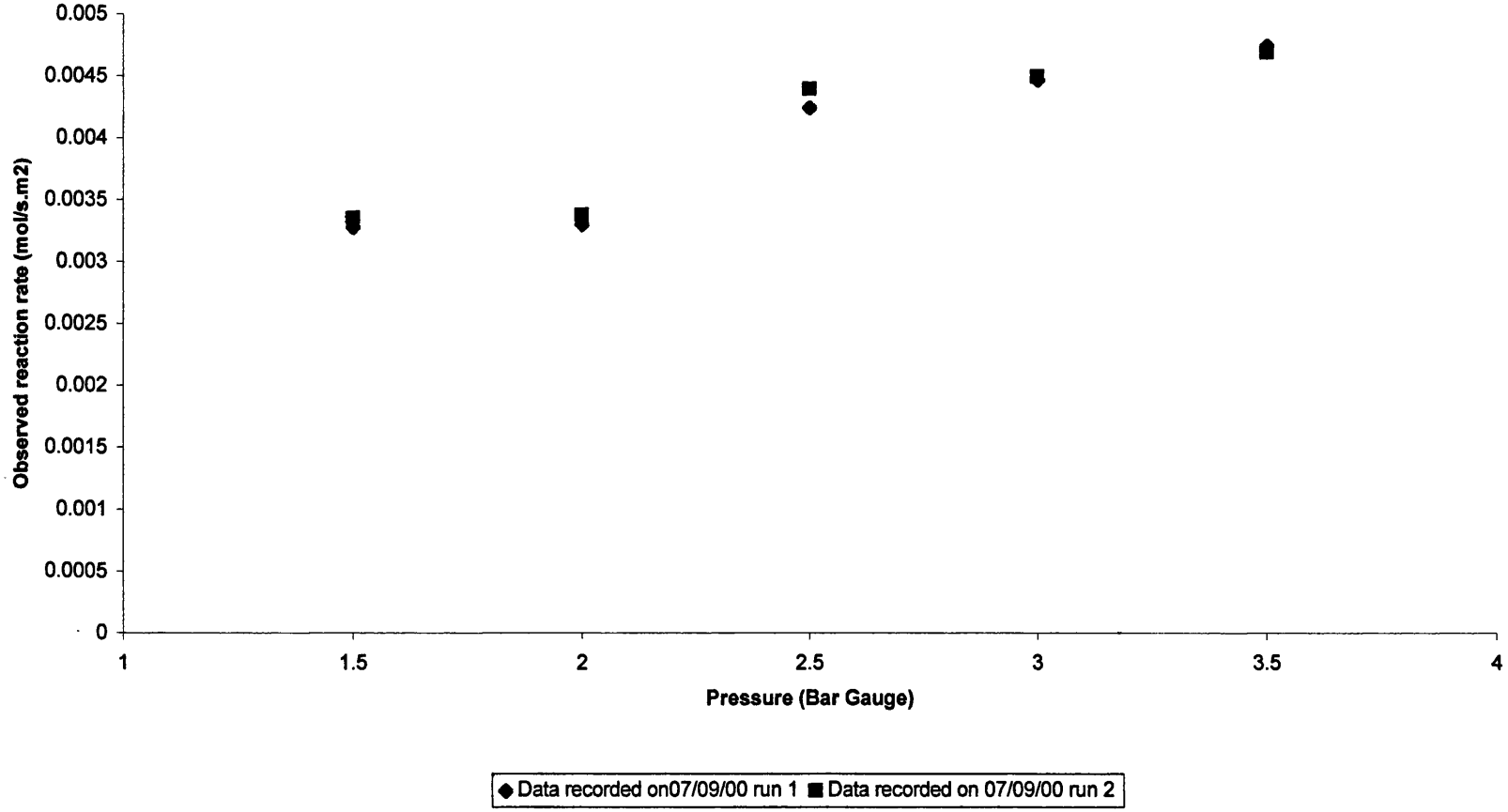
Graph 6.3: Effect of pressure on the catalytic combustion of Diesel over Platinum (4g Active phase per litre of monolith), at a constant throughput and a constant inlet setpoint temperature of 500°C



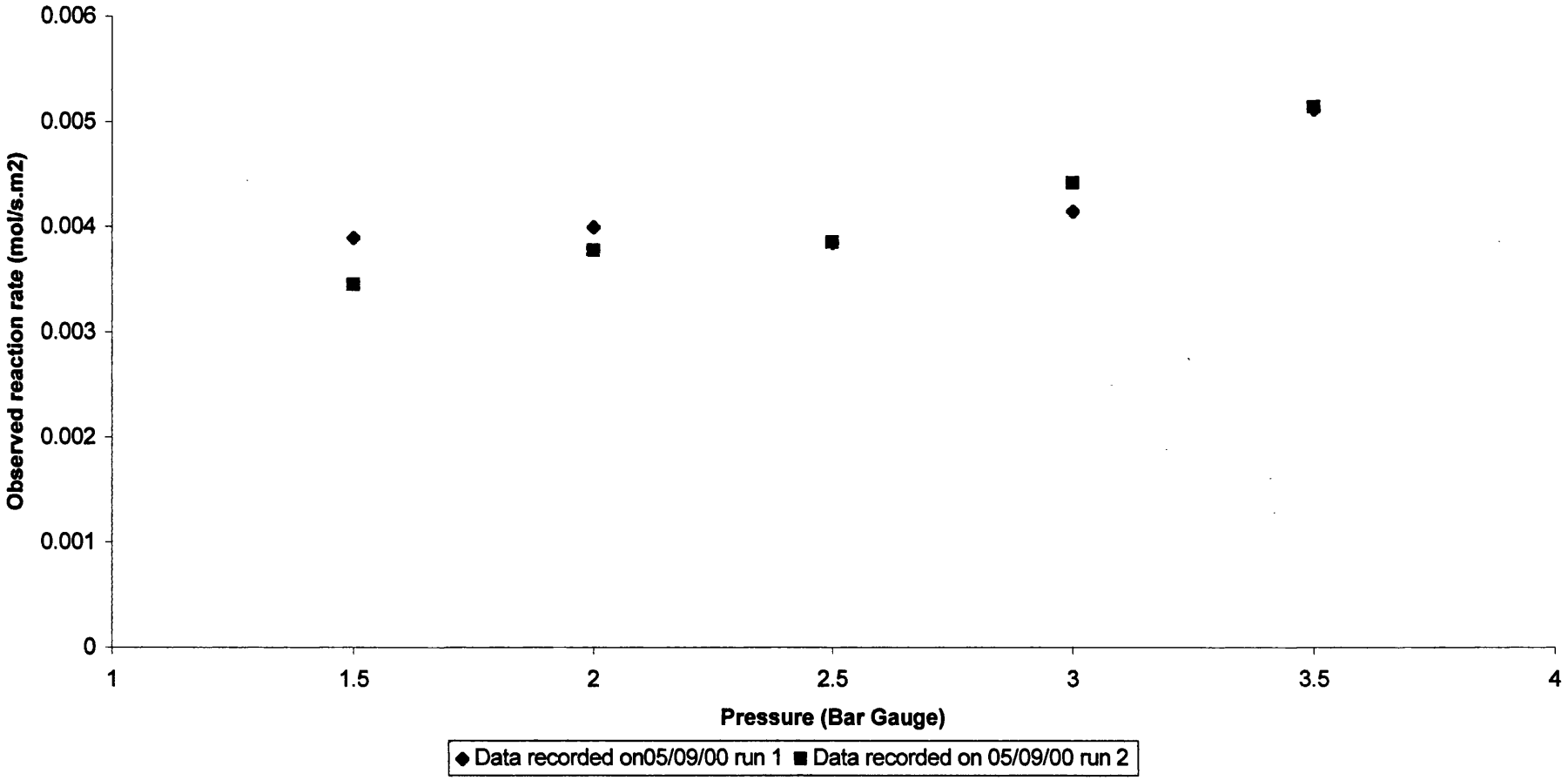
Graph 6.4: Effect of pressure on the catalytic combustion of Diesel over Platinum (8g Active phase per litre of monolith), at a constant throughput and a constant inlet setpoint temperature of 500°C



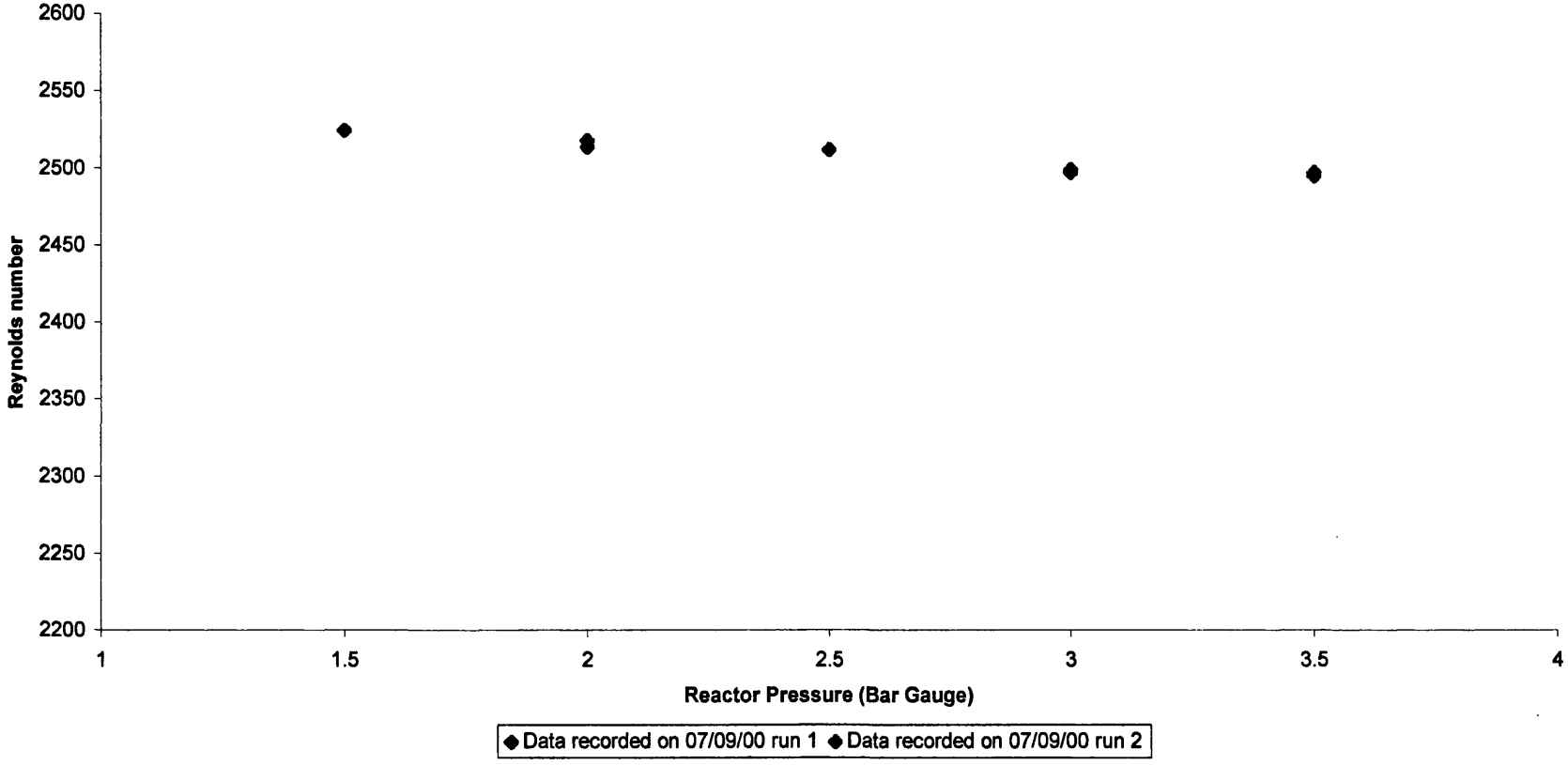
Graph 6.5: Effect of pressure on the catalytic combustion of Diesel over Platinum (4g Active phase per litre of monolith), at a constant throughput and a constant inlet setpoint temperature of 500°C



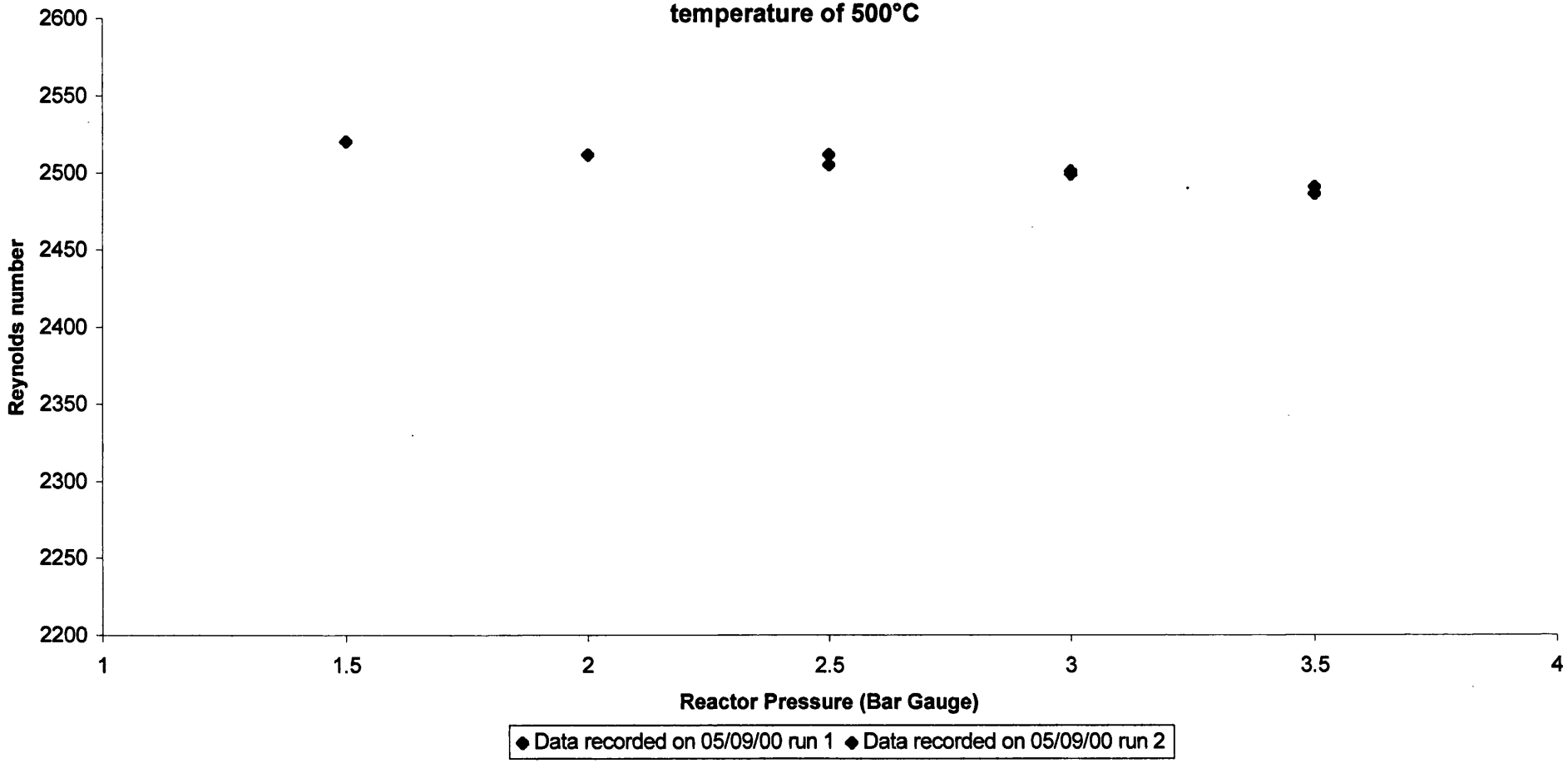
Graph 6.6: Effect of pressure on the catalytic combustion of Diesel over Platinum (8g Active phase per litre of monolith), at a constant throughput and a constant inlet setpoint temperature of 500°C



Graph 6.7: Reynolds number against reactor pressure for the catalytic combustion of diesel fuel over Platinum (4g active phase per litre of monolith), at constant throughput and constant inlet setpoint temperature of 500°C



Graph 6.8: Reynolds number against reactor pressure for the catalytic combustion of diesel fuel over Platinum (8g active phase per litre of monolith), at constant throughput and constant inlet setpoint temperature of 500°C



6.1.3 Fuel flowrate effects

In these experiments the effect of changing the fuel flowrate on the catalytic combustion of Diesel fuel was investigated. All other conditions in the test rig were fixed. The platinum catalysts were assembled into the test rig as described in the Chapter 4. The flowrate of air through the rig was fixed for each fuel flowrate to 500 litres/min, (Chapter 4), (Evaluated at 20°C and 1 bar pressure). The Diesel fuel was pumped into the test rig using a metering pump and varied. The range of fuel flowrates studied was 2.8, 4.2, 5.6 and 7.0 ml/min (Evaluated at 20°C and 1 bar pressure). The reactor inlet temperature was fixed at 500°C, and the pressure in the reactor was maintained constant at 2.0 barg. For each different fuel flowrate the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in the Chapter 3. The results can be found in Appendix G.

From the raw experimental results, values for the observed reaction rate could be calculated as shown previously in Chapter 5. These calculated results are included with the raw experimental results in Appendix G.

Graphs of the observed reaction rate against the fuel flowrate were then plotted for both the platinum catalysts studied (*Graph 6.9 and 6.10*), and are shown at the end of this section

From the graph the following conclusions can be drawn:

1. The observed rate of reaction increased with an increase in the Diesel fuel flowrate. At a Diesel flowrate of 2.6 ml/min the observed reaction rate was $3.3x10^{-3}$ mol/s m^2 for the platinum catalyst with 4 g active phase per litre of monolith and $1.6x10^{-3}$ mol/s m^2 for the platinum catalyst with 8 g active phase per litre of monolith. At a Diesel flowrate of 7.0 ml/min the observed rate of reaction had increased to a value of approx $3.3x10^{-3}$ mol/s m^2 for the platinum catalyst with 4 g active phase per litre of monolith and $4.0x10^{-3}$ mol/s m^2 for the platinum catalyst with 8 g active phase per litre of monolith.

The catalytic combustion of Diesel fuel is dependant on the Diesel flowrate. Doubling the amount of platinum active phase on the catalysts has little effect on the observed rates of reaction

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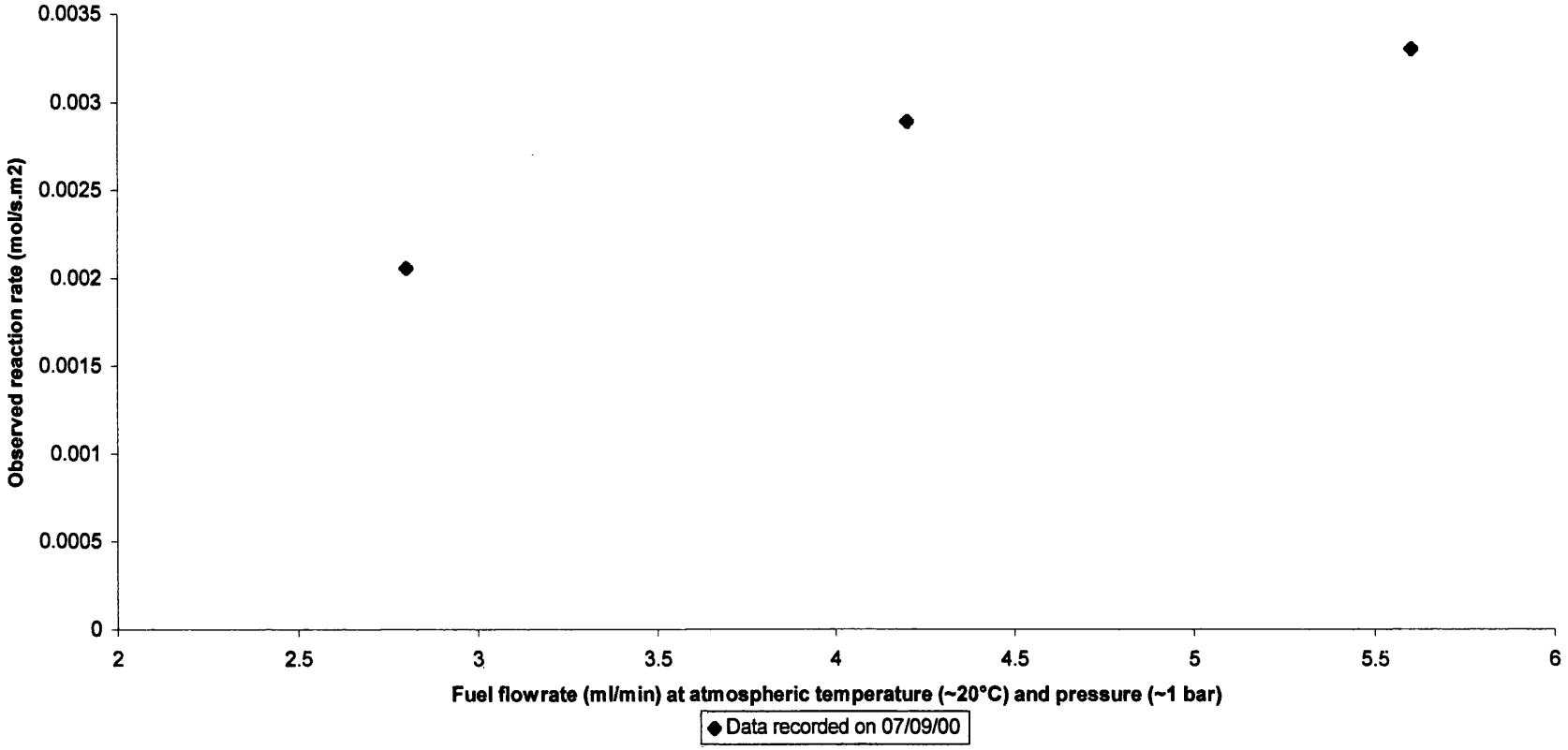
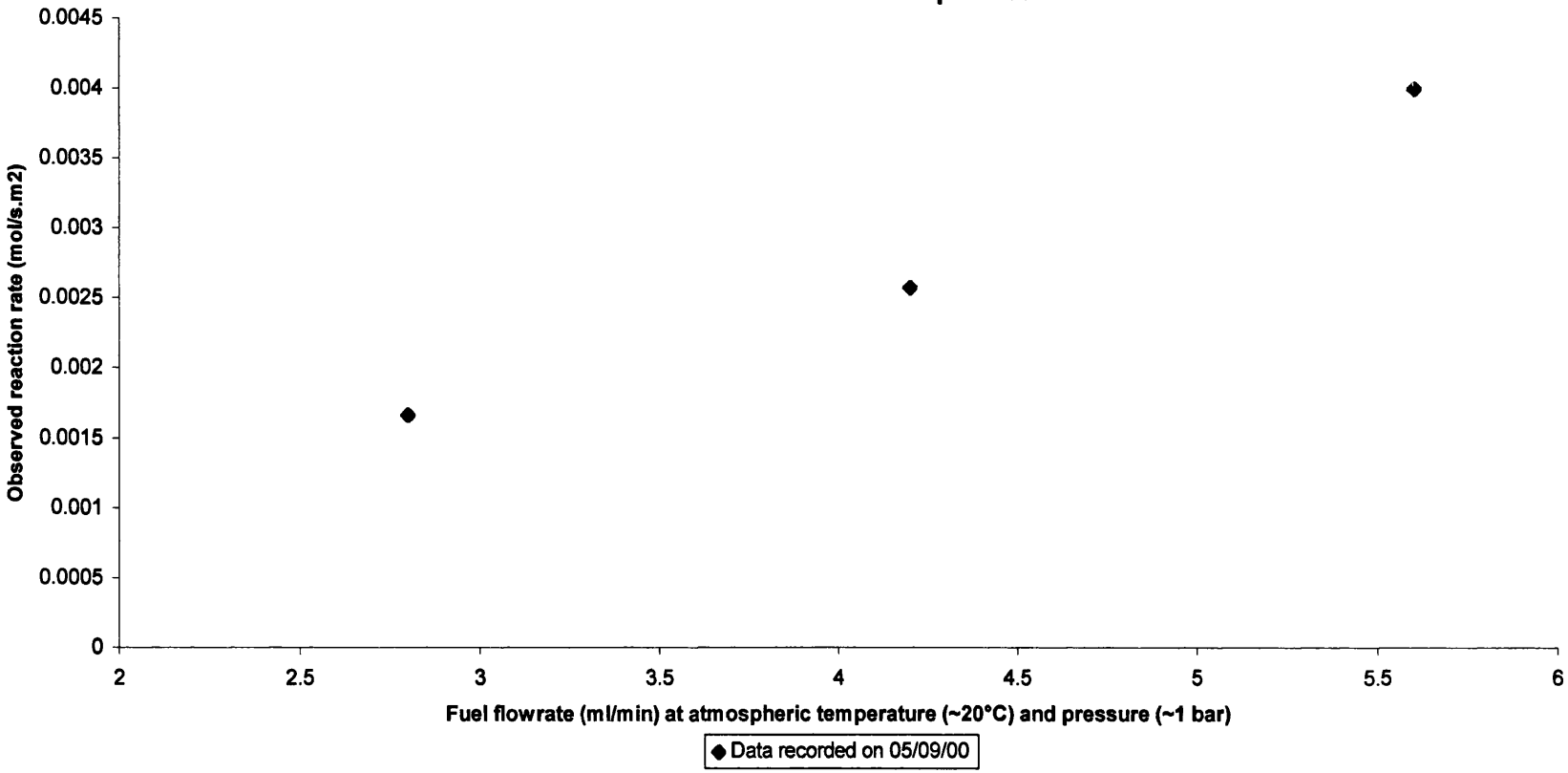
Graph 6.9: Effect of changing Fuel flowrate on the catalytic combustion of Diesel fuel over Platinum catalyst (4g Active phase per litre of monolith) at constant pressure of 2 bar gauge, constant air flowrate of 500 l/min and constant inlet temp of 500°C



Graph 6.10:Effect of changing Fuel flowrate on the catalytic combustion of Diesel fuel over Platinum catalyst (8g Active phase per litre of monolith) at constant pressure of 2 bar gauge, constant air flowrate of 500 l/min and constant inlet temp of 500°C



6.1.4 Total mass flowrate effects.

In these experiments the effect of changing the total mass flowrate on the catalytic combustion of Diesel fuel was investigated. All other conditions in the test rig were fixed. The catalysts were assembled into the test rig as described in the Chapter 4. The flowrate of air through the rig was varied along with the Diesel fuel flowrate such that at each total flowrate studied the air to fuel ratio (mol basis) remained constant at 872.7. The ranges of air and Diesel fuel flowrates studied are shown in the following table. All flowrates were recorded at atmospheric temperature and pressure (20°C and 1 bar.)

Air flowrate (l/min)	Diesel flowrate (ml/min)	Air to Fuel ratio (mol basis)	Equivalence Ratio
250	2.8	872.7	0.008
500	5.6	872.7	0.008
750	8.4	872.7	0.008

Experiments were performed at fixed pressures of 2.0 barg and then repeated at 3.5 barg. The reactor inlet set temperature was fixed at 400°C, and the experiments were then repeated for inlet set temperatures of 450°C and 500°C, at both the fixed pressures of 2.0 barg and 3.5 barg. For each different total flowrate the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in Chapter 3. The results can be found in Appendix G.

From the raw experimental results, values for the observed reaction rate could be calculated as shown previously in the Chapter 5. These calculated results are included with the raw experimental results in Appendix G.

Graphs of the observed reaction rate against the total mass flowrate for both set pressures and inlet temperatures were then plotted for both catalysts (*Graphs 6.11 and 6.12*), and are shown at the end of this section.

From the graphs the following conclusions can be drawn:

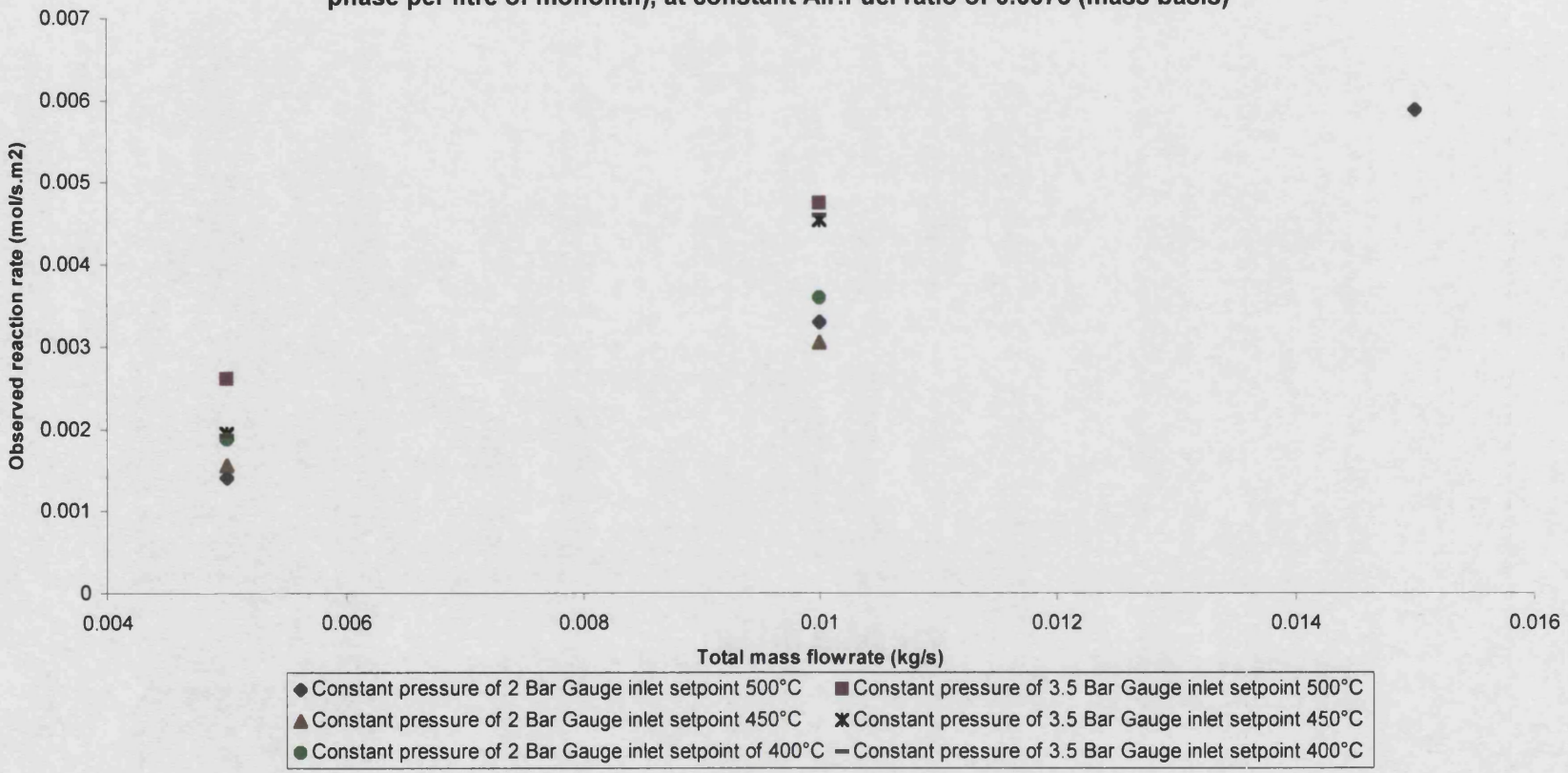
For the 4 g active phase per litre of monolith catalyst

1. The observed rate of reaction increases with an increase in the total mass flowrate. This indicates that the catalytic combustion is mass transfer limited even through the flowrate is transitional through a channel.
2. The trend is repeated for both pressures, and all of the inlet temperatures studied.
3. At the largest total mass flowrate studied (0.015 kg/s), the observed reaction rate is highest for a reactor pressure of 2 barg and inlet temperature set point of 500°C (6.0×10^{-3} mol/s m^2), and is lowest for a reactor pressure of 2 barg and inlet set point of 500°C (1.5×10^{-3} mol/s m^2).
4. At the lowest total mass flowrate studied (0.005 kg/s), the observed reaction rate is highest for a reactor pressure of 3.5 barg and inlet temperature set point of 500°C (2.5×10^{-3} mol/s m^2), and is lowest for a reactor pressure of 2.0 barg and constant with temperature at 1.5×10^{-3} mol/s m^2

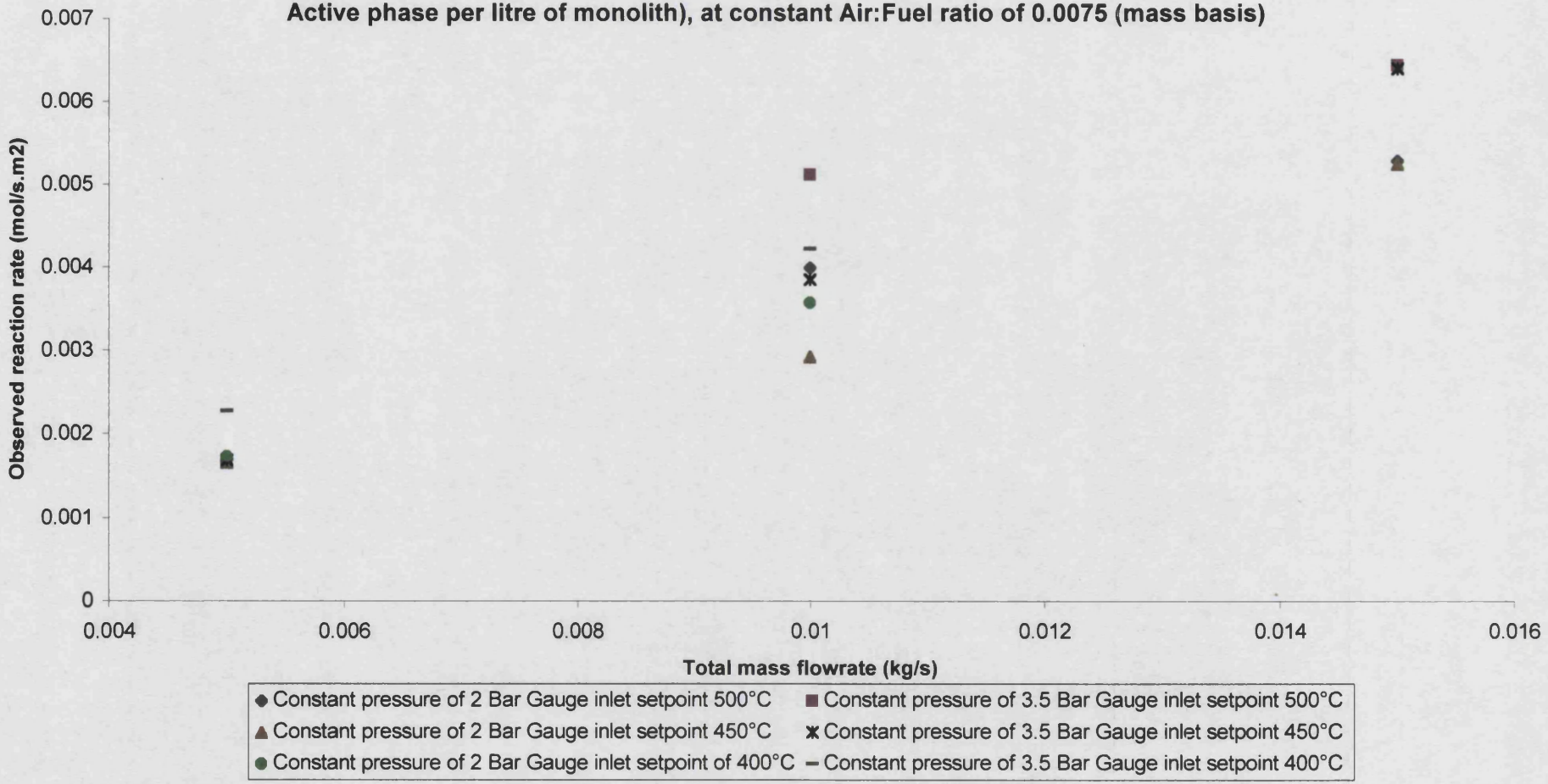
For the 8 g active phase per litre of monolith catalyst

1. The observed rate of reaction increases with an increase in the total mass flowrate. This indicates that the catalytic combustion is mass transfer limited even through the flowrate is turbulent through a channel.
2. The trend is repeated for both pressures, and all of the inlet temperatures studied.
3. At the largest total mass flowrate studied (0.015 kg/s), the observed reaction rate is highest for a reactor pressure of 3.5 barg and inlet temperature set point of 500°C (6.5×10^{-3} mol/s m^2), and is lowest for a reactor pressure of 2 barg and inlet set point of 450°C (5.0×10^{-3} mol/s m^2).
4. At the lowest total mass flowrate studied (0.005 kg/s), the observed reaction rate is highest for a reactor pressure of 3.5 barg and inlet temperature set point of 400°C (2.2×10^{-3} mol/s m^2), and is lowest for a reactor pressure of 2.0 barg and inlet set point temperature of 400°C (1.7×10^{-3} mol/s m^2).

Graph 6.11: Effect of total mass flowrate on the catalytic combustion of Diesel fuel over Platinum (4g Active phase per litre of monolith), at constant Air:Fuel ratio of 0.0075 (mass basis)



Graph 6.12: Effect of total mass flowrate on the catalytic combustion of Diesel fuel over Platinum (8g Active phase per litre of monolith), at constant Air:Fuel ratio of 0.0075 (mass basis)



6.2 Results for the Catalytic Combustion of Diesel Fuel over $LaMnO_3$ Perovskite type Catalysts.

Experiments were performed using $LaMnO_3$ perovskite type catalysts of fixed dimensions. All monoliths had an initial gamma alumina washcoat layer of approx 110 g alumina per litre of monolith, which were calcinated to 500°C. The Perovskite active phase of $LaMnO_3$ was added to give finial catalysts with approx 24 g $LaMnO_3$ per litre of monolith, and 8 g $LaMnO_3$ per litre of monolith. The finished catalysts were calcinated to 800°C. Full details on the production of the catalysts can be found in the Chapter 4.

6.2.1 Inlet Temperature effects.

In these experiments the effect of changing the catalyst inlet temperature on the catalytic combustion of Diesel fuel was investigated. All other conditions in the test rig were fixed. The perovskite catalysts were assembled into the test rig as described in the Chapter 4. The flowrate of air through the rig was fixed at 500 litres/min (Evaluated at 20°C and 1 bar pressure). The Diesel fuel was pumped into the test rig using a metering pump at a fixed rate of 5.6 ml/min, (Chapter 4), (Evaluated at 20°C and 1 bar pressure). The reactor pressure was fixed at 2 barg using a back-pressure control valve. The catalyst inlet temperature was varied by altering the electric air heater set point from 350°C to 500°C in increments of 50°C. At each different temperature set point the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in the Chapter 3. The experiments were repeated twice recorded as run 1 and run 2 respectively. The results can be found in Appendix H.

From the raw experimental results, values for the observed reaction rate were calculated as described in Chapter 5.

Graphs were then plotted of the observed reaction rate against the actual inlet temperature to the reactor for the perovskite catalysts (*Graphs 6.13 and 6.14*). These are shown at the end of this section

From the graphs the following conclusions can be drawn:

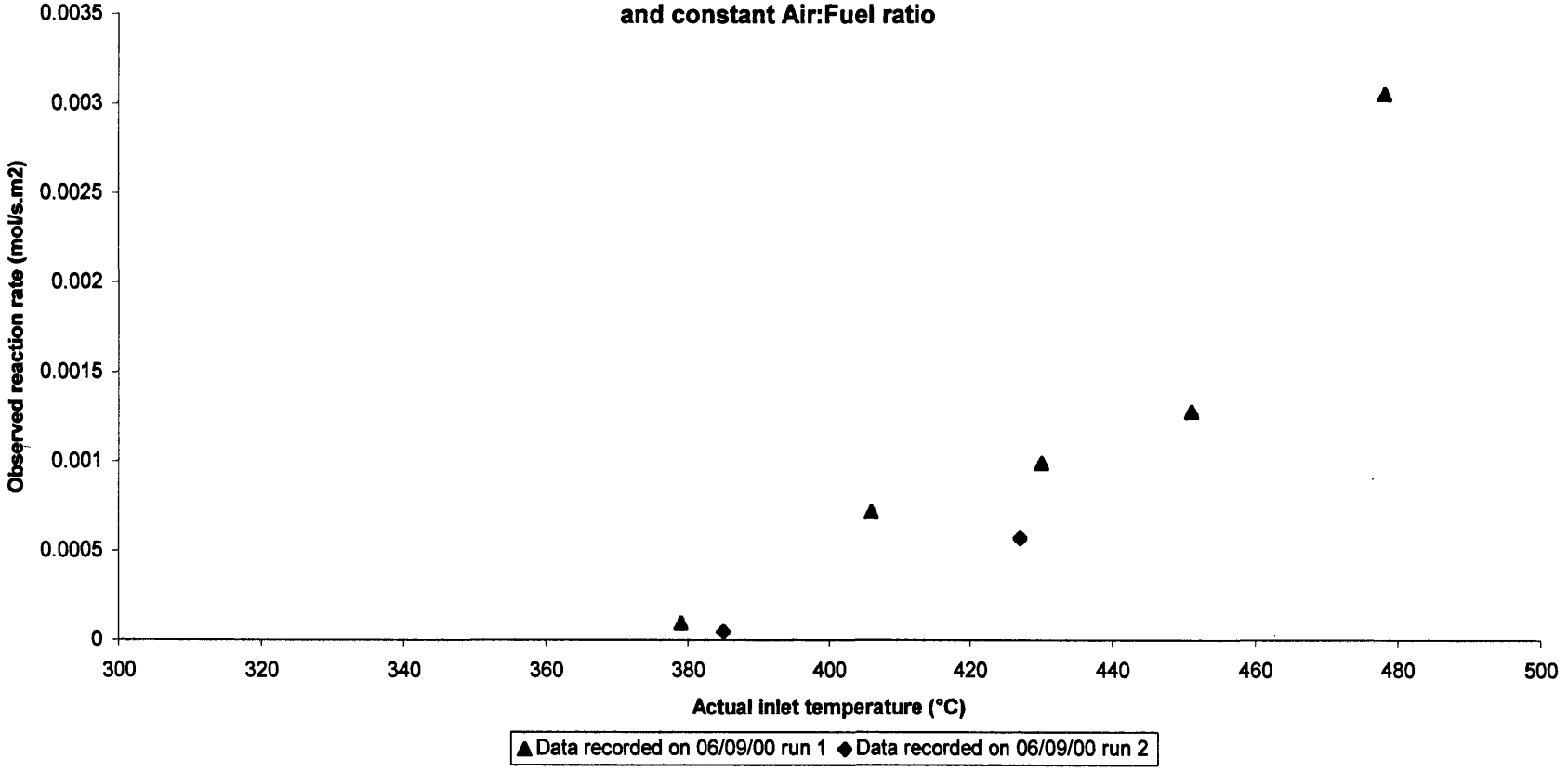
For the 8 g active phase per litre of monolith catalyst

1. The catalyst shows no activity for the combustion of diesel fuel at inlet temperatures of below 380°C. The observed rate of reaction then increases with inlet temperature to a value of 3.1×10^{-3} mol/s m^2 at an inlet temperature of 480°C.
2. The results are repeatable as the values of the observed rate of reaction for run 1 and run 2 are in good agreement.

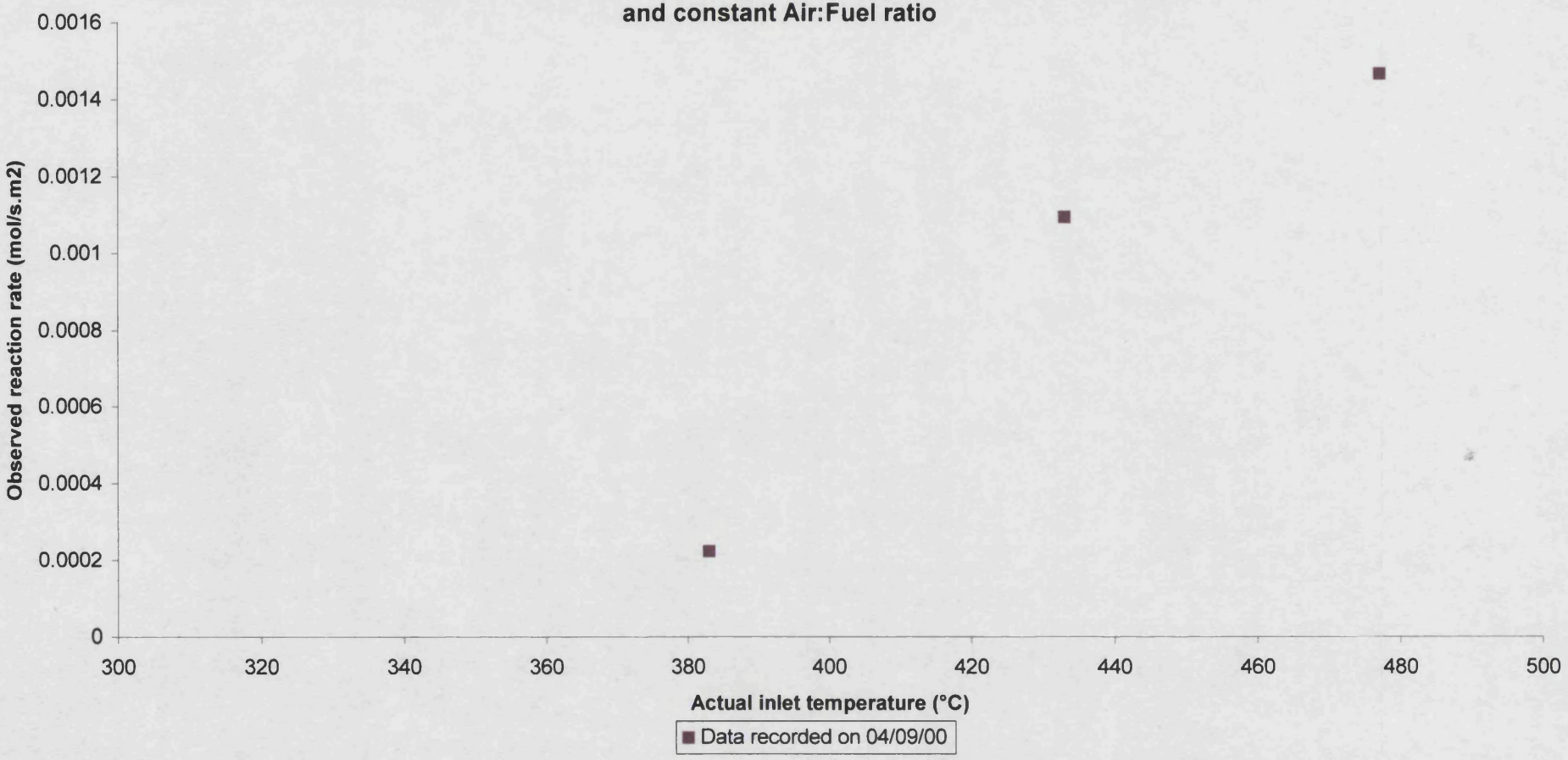
For the 24 g active phase per litre of monolith catalyst

The catalyst shows no activity for the combustion of diesel fuel at inlet temperatures of below 380°C. The observed rate of reaction then increases with inlet temperature to a value of 1.5×10^{-3} mol/s m^2 at an inlet temperature of 480°C.

Graph 6.13: Temperature conversion chart for the catalytic combustion of Diesel fuel over LaMnO3 perovskite (8g Active phase per litre of monolith), at constant pressure of 2 bar gauge, constant mass flow and constant Air:Fuel ratio



Graph 6.14: Temperature conversion chart for the catalytic combustion of Diesel fuel over LaMnO3 perovskite (24g Active phase per litre of monolith), at constant pressure of 2 bar gauge, constant mass flow and constant Air:Fuel ratio



6.2.2 Pressure Effects

In these experiments the effect of changing the reactor pressure on the catalytic combustion of Diesel fuel was investigated. All other conditions in the test rig were fixed. The perovskite catalysts were assembled into the test rig as described in the Chapter 4. The flowrate of air through the rig was fixed at each different pressure to 500 litres/min (Evaluated at 20°C and 1 bar pressure). The Diesel fuel was pumped into the test rig using a metering pump at a fixed rate of 5.6 ml/min, (Chapter 4), (Evaluated at 20°C and 1 bar pressure). The reactor inlet temperature was fixed at 500°C. The pressure in the reactor was varied by adjusting the back-pressure control valve to give pressures varying from 1.5 barg up to 3.5 barg in intervals of 0.5 barg. At each different pressure set point the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in the Chapter 3. The experiments were repeated twice and recorded as run 1 and run 2 respectively. The results can be found in Appendix H.

From the raw experimental results, values for the observed reaction rate were calculated as shown previously in Chapter 5. These calculated results are included with the raw experimental results in Appendix H.

Values for the Reynolds number through a channel were also calculated from the experimental results as described in Chapter 5. These results are also included in Appendix H.

Having calculated the observed reaction rate and Reynolds number through a channel for each pressure studied the following graphs were plotted:

1. The temperature rise across the catalysts against reactor pressure for both Perovskite catalysts (*Graphs 6.15 and 6.16*).
2. The Observed reaction rate against reactor pressure for both Perovskite catalysts (*Graphs 6.17 and 6.18*).
3. The Reynolds number through a channel against reactor pressure for both Perovskite catalysts (*Graphs 6.19 and 6.20*).

These graphs are all shown at the end of this section.

From the graphs the following conclusions can be drawn:

Perovskite Catalyst with 8 g active phase per litre of monolith

1. As the pressure is increased from 1.5 barg to 2 barg the temperature rise across the reactor increases from approx 30°C to approx 90°C.
2. The observed reaction rate increases with pressure. At 1.5 barg the reaction rate is approx 7.0×10^{-4} mol/s.m^2. This rises to a value of 2.5×10^{-3} mol/s m^2 at 3.5 barg. This shows that the rate of reaction of Diesel fuel is affected by pressure. The higher values of pressure give a larger observed reaction rate hence more of the available Diesel fuel is combusted.
3. The Reynolds number through a channel remains approximately constant with pressure at 2500. This indicates Transitional flow through the channels, and that the observed increase in reaction rate noticed with increasing pressure is not a result of changes in the Reynolds number.
4. All the results are repeatable as both run 1 and run 2 are in close agreement.

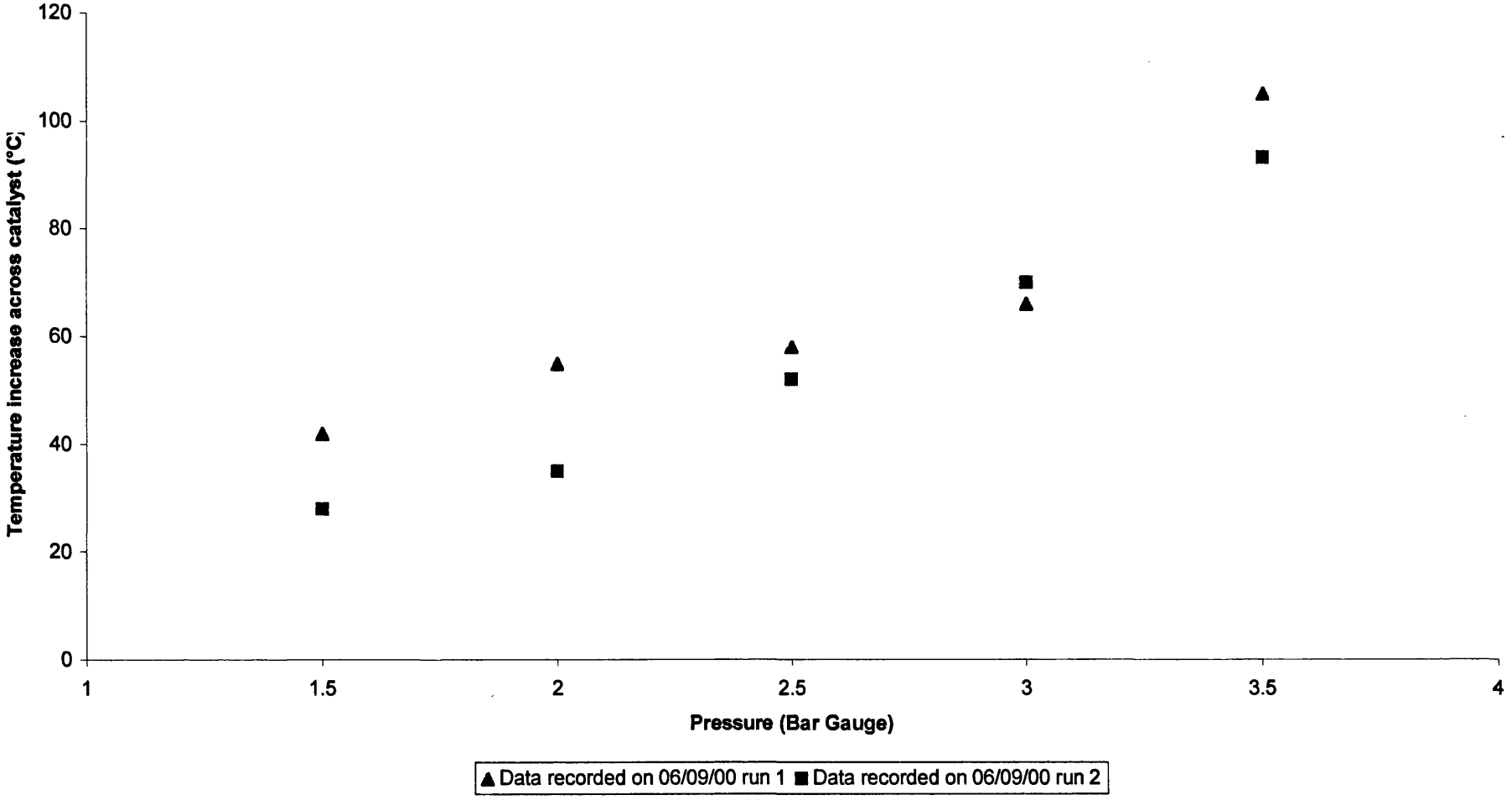
Perovskite Catalysts with 24 g active phase per litre of monolith

1. As the pressure is increased from 1.5 barg to 3.5 barg the temperature rise across the reactor increases from approx a 50°C to a 95°C rise at 3.5 barg. This indicates that more of the Diesel fuel present in the air is being combusted at the higher pressures.
2. The observed reaction rate also changes with pressure. At 1.5 barg the observed reaction rate is approx $1.3x10^{-3}$ mol/s m^2. The observed reaction rate then increases with pressure to a value of approx $2.5x10^{-3}$ mol/s m^2 at 3.5 barg
3. The Reynolds number through a channel shows minor fluctuations with pressure, but is approx constant at 2500 over the range of pressures studied. This indicates Transitional flow through the channels, and that the observed changes in the rate of reaction noticed with increasing pressure is not a result of changes in the Reynolds number.
4. All the results are repeatable as both run 1 and run 2 are in close agreement.

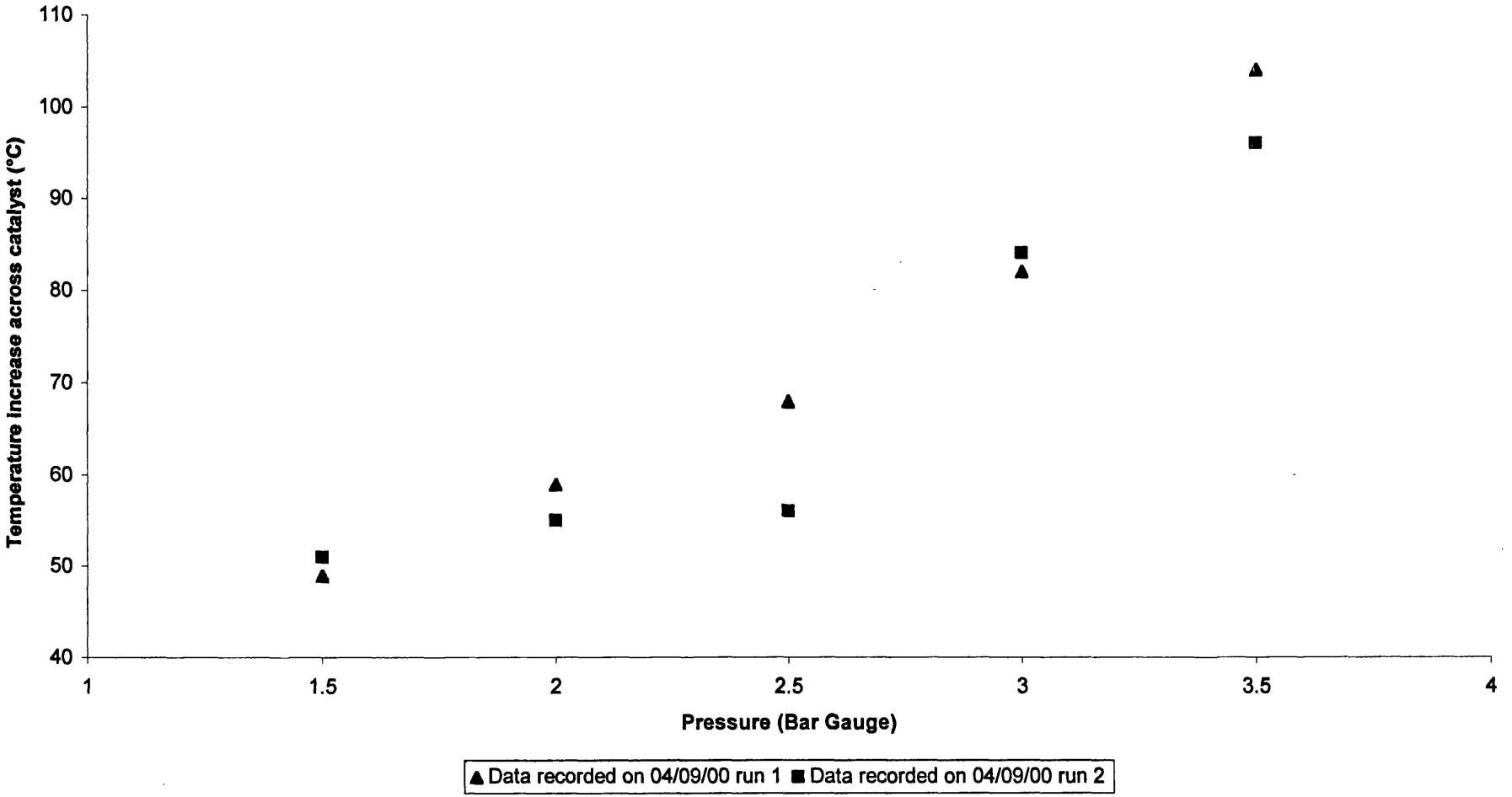
Overall conclusions

1. The Observed rate of reaction is dependent on the reactor pressure. Higher pressures show an increase in the observed rate of reaction, which is also shown by an increase in the temperature rise across the catalyst bed.
2. Trebling the amount of perovskite active phase on the catalyst shows no effect on the temperature rise across the reactor
3. Trebling the amount of perovskite active phase on the catalyst increases the observed rate of reaction by a factor of 1.86 at 1.5 barg and has no affect at 3.5 barg.
4. The Reynolds numbers through a channel remain unchanged with reactor pressure, and are similar for both the perovskite catalysts at approx 2500.

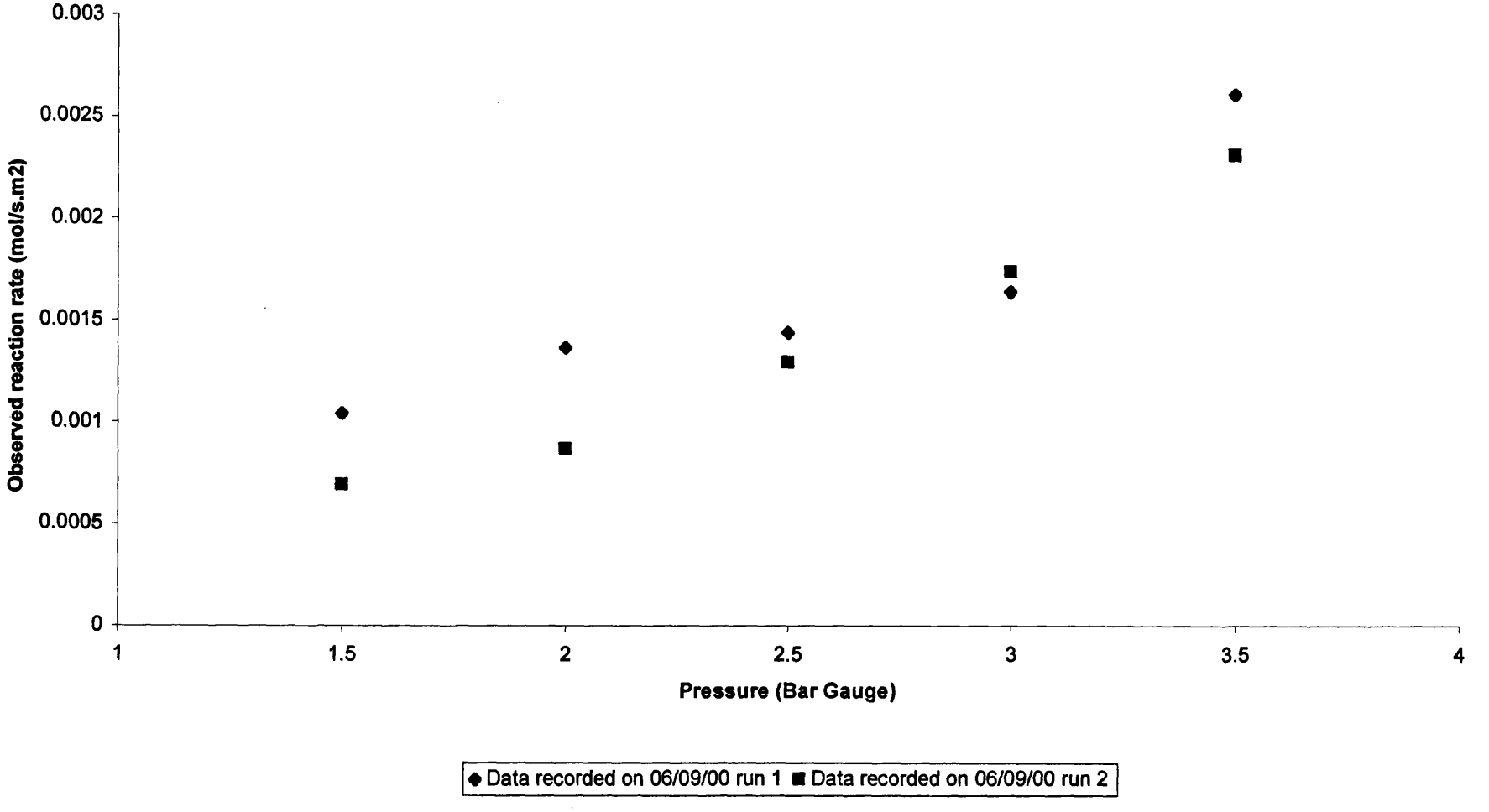
Graph 6.15: Effect of pressure on the catalytic combustion of Diesel over LaMnO3 perovskite (8g Active phase per litre of monolith), at a constant throughput and a constant inlet setpoint temperature of 500°C



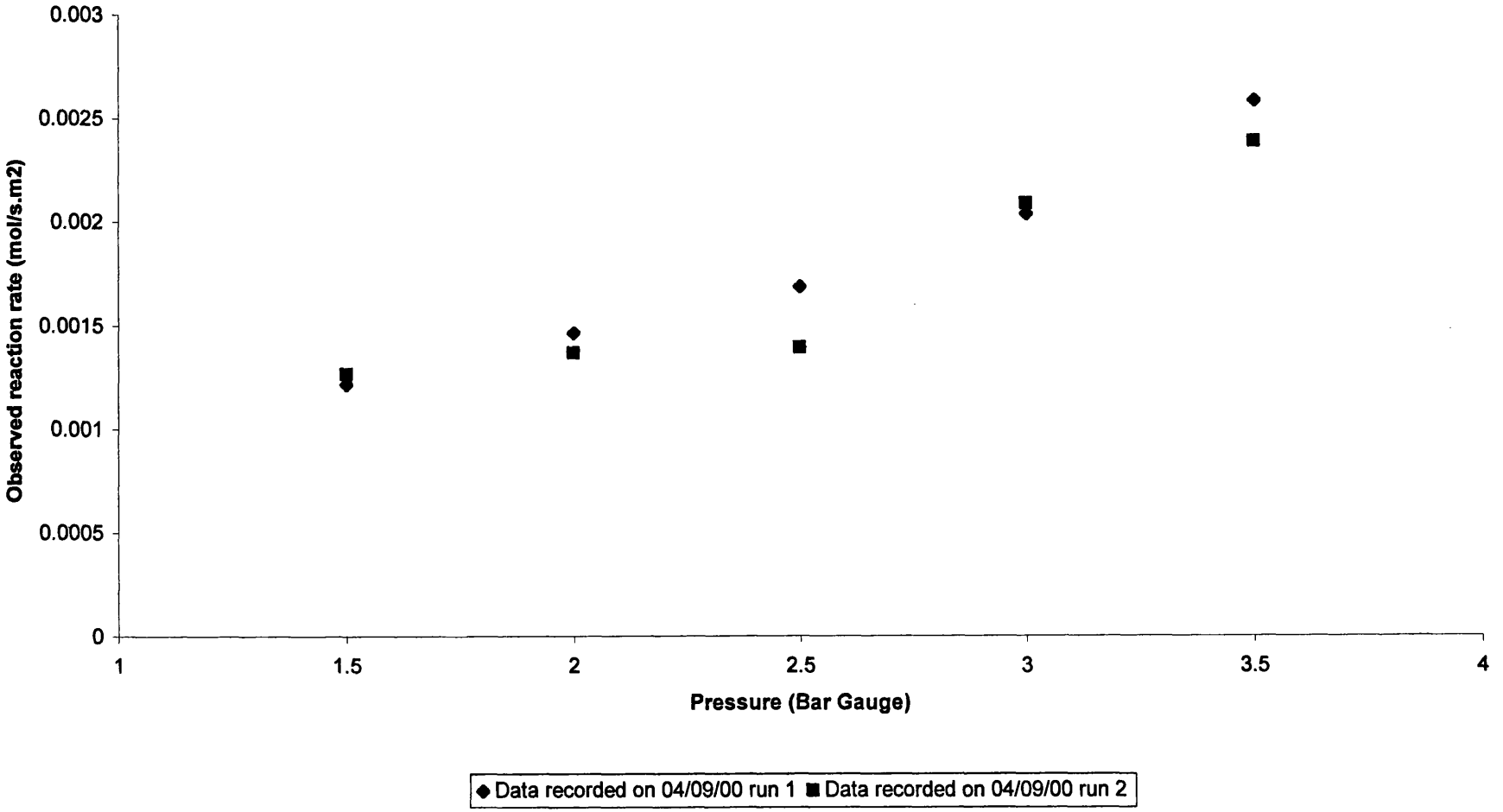
Graph 6.16: Effect of pressure on the catalytic combustion of Diesel over LaMnO3 perovskite (24g Active phase per litre of monolith), at a constant throughput and a constant inlet setpoint temperature of 500°C



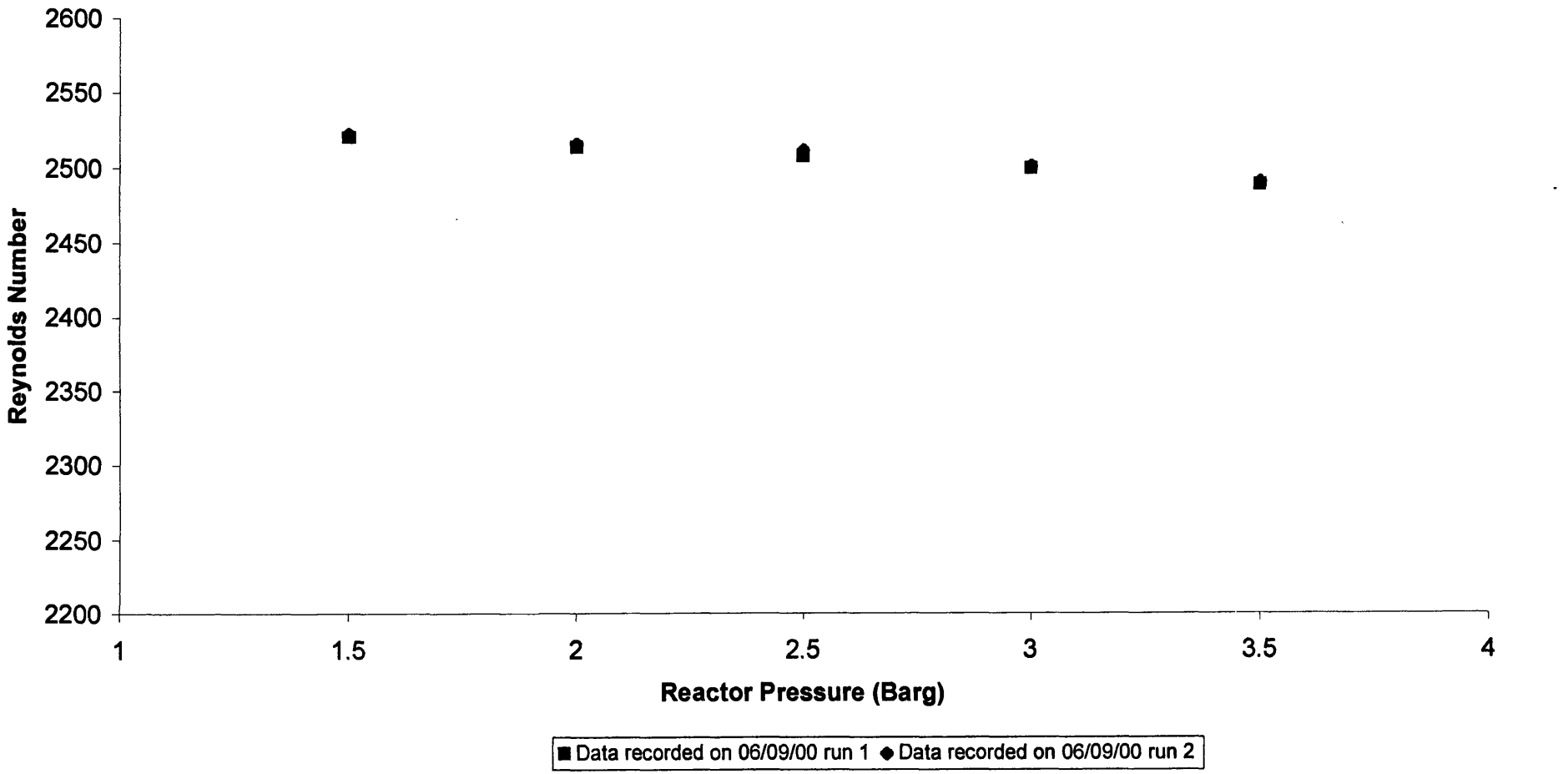
Graph 6.17: Effect of pressure on the catalytic combustion of Diesel over LaMnO3 perovskite (8g Active phase per litre of monolith), at a constant throughput and a constant inlet setpoint temperature of 500°C



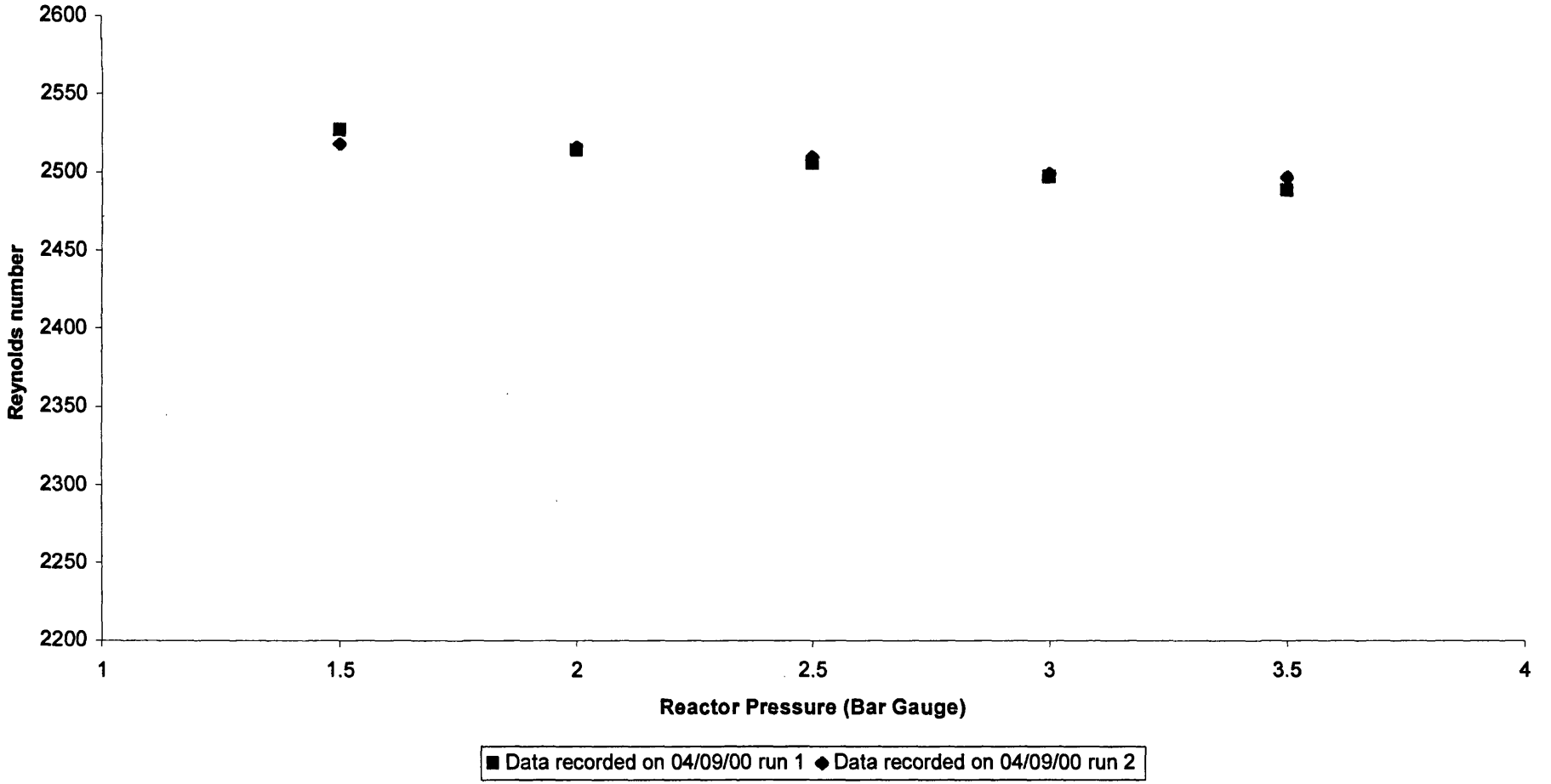
Graph 6.18: Effect of pressure on the catalytic combustion of Diesel over LaMnO3 perovskite (24g Active phase per litre of monolith), at a constant throughput and a constant inlet setpoint temperature of 500°C



Graph 6.19: Reynolds number against reactor pressure for the catalytic combustion of diesel fuel over perovskite LaMnO3 (8g active phase per litre of monolith), at constant throughput and constant inlet setpoint temperature of 500°C



Graph 6.20: Reynolds number against reactor pressure for the catalytic combustion of diesel fuel over perovskite LaMnO3 (24g active phase per litre of monolith), at constant throughput and constant inlet setpoint temperature of 500°C



6.2.3 Fuel flowrate effects

In these experiments the effect of changing the fuel flowrate on the catalytic combustion of Diesel fuel was investigated. All other conditions in the test rig were fixed. The perovskite catalysts were assembled into the test rig as described in Chapter 4. The flowrate of air through the rig was fixed for each fuel flowrate to 500 litres/min (Evaluated at 20°C and 1 bar pressure). The Diesel fuel was pumped into the test rig using a metering pump and varied. The range of fuel flowrates studied was 2.8, 4.2, 5.6 and 7.0 ml/min (Evaluated at 20°C and 1 bar pressure). The reactor inlet temperature was fixed at 500°C, and the pressure in the reactor was maintained constant at 2.0 barg. For each different fuel flowrate the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in Chapter 3. The results can be found in Appendix H.

From the raw experimental results, values for the observed reaction rate could be calculated as shown previously in Chapter 5. These calculated results are included with the raw experimental results in Appendix H.

Graphs of the observed reaction rate against the fuel flowrate were then plotted, for each of the perovskite catalysts (*Graphs 6.21 and 6.22*), and are shown at the end of this section.

From the graphs the following conclusions can be drawn:

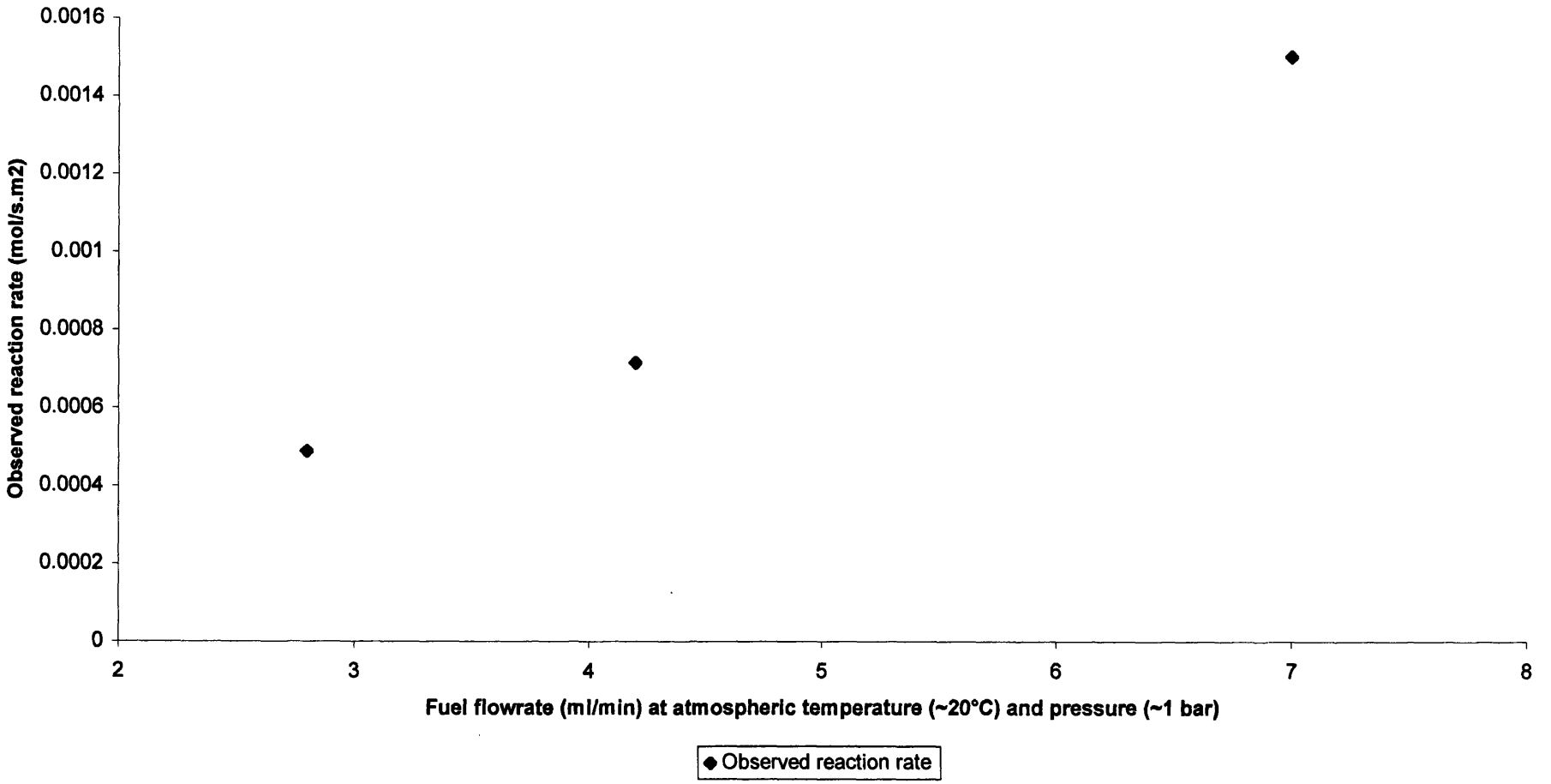
For the 8 g active phase per litre of monolith catalyst:

The observed rate of reaction increased with an increase in the Diesel fuel flowrate. At a Diesel flowrate of 2.6 ml/min the observed reaction rate was $5.0x10^{-4}$ mol/s m^2. At a Diesel flowrate of 7.0 ml/min the observed rate of reaction had increased to a value of approx $1.5x10^{-3}$ mol/s m^2

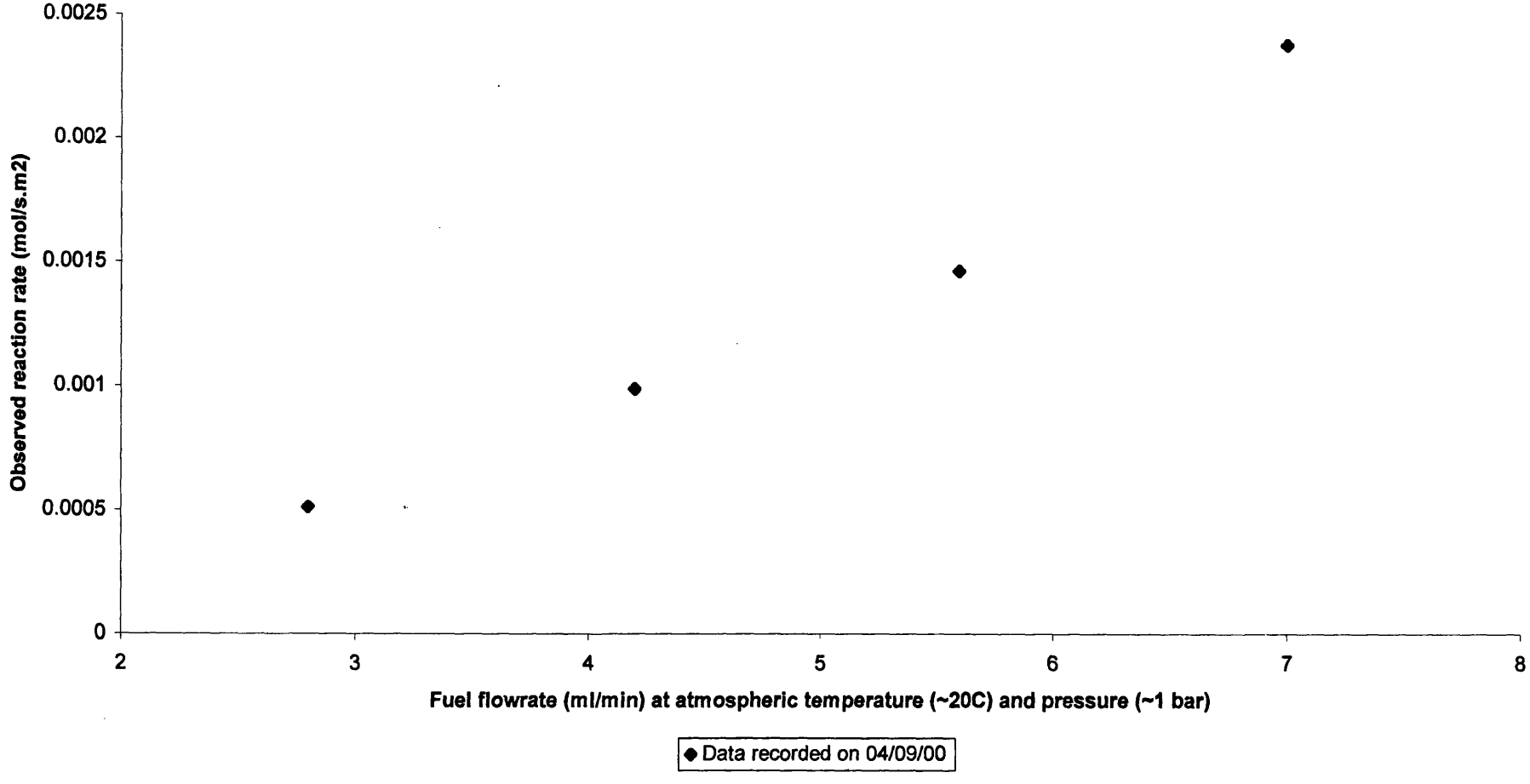
For the 24 g active phase per litre of monolith catalyst:

The observed rate of reaction increased with an increase in the Diesel fuel flowrate. At a Diesel flowrate of 2.6 ml/min the observed reaction rate was $5.0x10^{-4}$ mol/s m^2. At a Diesel flowrate of 7.0 ml/min the observed rate of reaction had increased to a value of approx $2.3x10^{-3}$ mol/s m^2

Graph 6.21: Effect of Fuel flowrate on the catalytic combustion of Diesel fuel over LaMnO3 perovskite catalyst (8g Active phase per litre of monolith) at constant pressure of 2 bar gauge, constant air flowrate of 500 l/min and constant inlet temp of 500°C



Graph 6.22: Effect ofFuel flowrate on the catalytic combustion of Diesel fuel over LaMnO3 perovskite catalyst (24g Active phase per litre of monolith) at constant pressure of 2 bar gauge, constant air flowrate of 500 l/min and constant inlet temp of 500°C



6.2.4 Total mass flowrate effects.

In these experiments the effect of changing the total mass flowrate on the catalytic combustion of Diesel fuel was investigated. All other conditions in the test rig were fixed. The catalysts were assembled into the test rig as described in the Chapter 4. The flowrate of air through the rig was varied along with the Diesel fuel flowrate such that at each total flowrate studied the air to fuel ratio remained constant at 872.7. The ranges of air and Diesel fuel flowrates studied are shown in the following table. All flowrates were recorded at atmospheric temperature and pressure (20°C and 1 bar.)

Air flowrate (l/min)	Diesel flowrate (ml/min)	Air: Fuel ratio (mol basis)	Equivalence Ratio
250	2.8	$1.1x10^{-5}$	0.008
500	5.6	$1.1x10^{-5}$	0.008
750	8.4	$1.1x10^{-5}$	0.008

Experiments were performed at fixed pressures of 2.0 barg and then repeated at 3.5 barg. The reactor inlet set temperature was fixed at 400°C, and the experiments were then repeated for inlet set temperatures of 450°C and 500°C, at both the fixed pressures of 2.0 barg and 3.5 barg. For each different total flowrate the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in Chapter 3. The results can be found in Appendix H.

From the raw experimental results, values for the observed reaction rate could be calculated as shown previously in Chapter 5. These calculated results are included with the raw experimental results in Appendix H.

Graphs of the observed reaction rate against the total mass flowrate for both set pressures and inlet temperatures were then plotted for both catalysts (*Graphs 6.23 and 6.24*), and are shown at the end of this section.

From the graphs the following conclusions can be drawn:

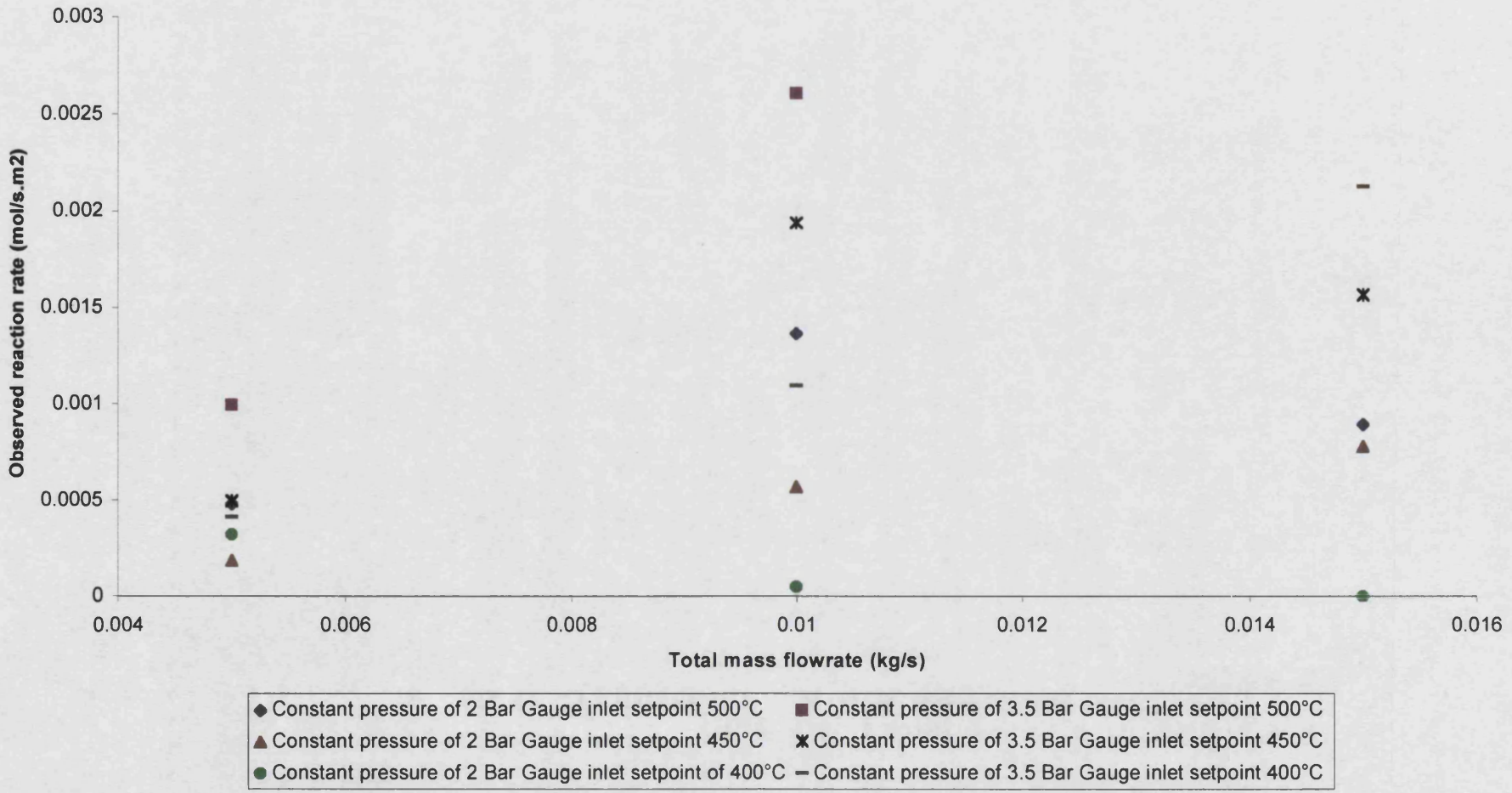
For the 8 g active phase per litre of monolith catalyst

1. The observed rate of reaction increases with an increase in the total mass flowrate. This indicates that the catalytic combustion is mass transfer limited even through the flowrate is transitional through a channel.
2. The trend is repeated for both pressures, and all of the inlet temperatures studied.
3. At the largest total mass flowrate studied (0.015 kg/s), the observed reaction rate is highest for a reactor pressure of 3.5 barg and inlet temperature set point of 400°C ($2.0x10^{-3}$ mol/s m^2), and is lowest for a reactor pressure of 2 barg and inlet set point of 400°C (>$0.5x10^{-3}$ mol/s m^2).
4. At the lowest total mass flowrate studied (0.005 kg/s), the observed reaction rate is highest for a reactor pressure of 3.5 barg and inlet temperature set point of 500°C ($1.0x10^{-3}$ mol/s m^2), and is lowest for a reactor pressure of 2 barg and inlet temperature set point of 450°C (>$0.5x10^{-3}$ mol/s m^2).

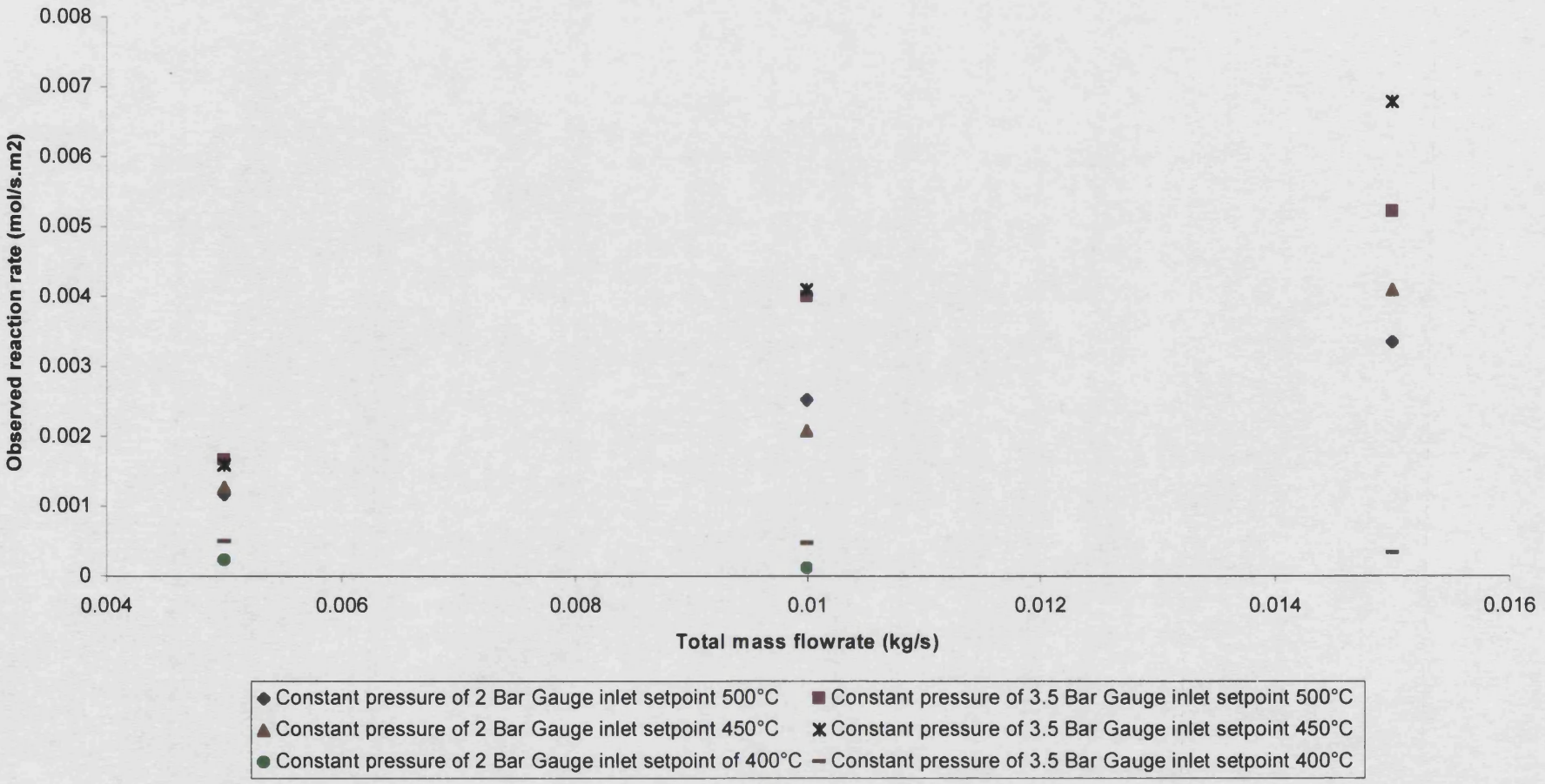
For the 24 g active phase per litre of monolith catalyst

1. The observed rate of reaction increases with an increase in the total mass flowrate. This indicates that the catalytic combustion is mass transfer limited even through the flowrate is turbulent through a channel.
2. The trend is repeated for both pressures, and all of the inlet temperatures studied.
3. At the largest total mass flowrate studied (0.015 kg/s), the observed reaction rate is highest for a reactor pressure of 3.5 barg and inlet temperature set point of 450°C (7.0×10^{-3} mol/s m^2), and is lowest for a reactor pressure of 3.5 barg and inlet set point of 400°C (5.0×10^{-4} mol/s m^2).
4. At the lowest total mass flowrate studied (0.005 kg/s), the observed reaction rate is highest for a reactor pressure of 3.5 barg and inlet temperature set point of 500°C (1.8×10^{-3} mol/s m^2), and is lowest for a reactor pressure of 2 barg and inlet set point temperature of 400°C ($>0.5 \times 10^{-4}$ mol/s m^2).

Graph 6.23: Effect of total mass flowrate on the catalytic combustion of Diesel fuel over LaMnO3 perovskite (8g Active phase per litre of monolith), at constant Air:Fuel ratio of 0.0075 (mass basis)



Graph 6.24: Effect of total mass flowrate on the catalytic combustion of Diesel fuel over LaMnO3 perovskite (24 g Active phase per litre of monolith), at constant Air:Fuel ratio of 0.0075 (mass basis). Data recorded on 02/09/00



6.3 Results for the Catalytic Combustion of Diesel Fuel over an industrial Catalyst supplied by Degussa.

Experiments were performed using an industrial catalyst supplied by Degussa. The active phase was disclosed as being platinum with a loading of approx 4 g platinum per litre of monolith. Full details on the Degussa catalyst can be found in the Chapter 4.

6.3.1 Inlet Temperature effects.

In these experiments the effect of changing the catalyst inlet temperature on the catalytic combustion of Diesel was investigated. All other conditions in the test rig were fixed. The Degussa catalyst was assembled into the test rig as described in Chapter 4. The flowrate of air through the rig was fixed at 500 litres/min (Evaluated at 20°C and 1 bar pressure). The Diesel fuel was pumped into the test rig using a metering pump at a fixed rate of 5.6 ml/min, (Chapter 4), (Evaluated at 20°C and 1 bar pressure). The reactor pressure was fixed at 2 barg using a back-pressure control valve. The catalyst inlet temperature was varied by altering the electric air heater set point from 350°C to 500°C in increments of 50°C. At each different temperature set point the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in Chapter 3. The experiment was repeated twice recorded as run 1 and run 2 respectively. The results can be found in Appendix I.

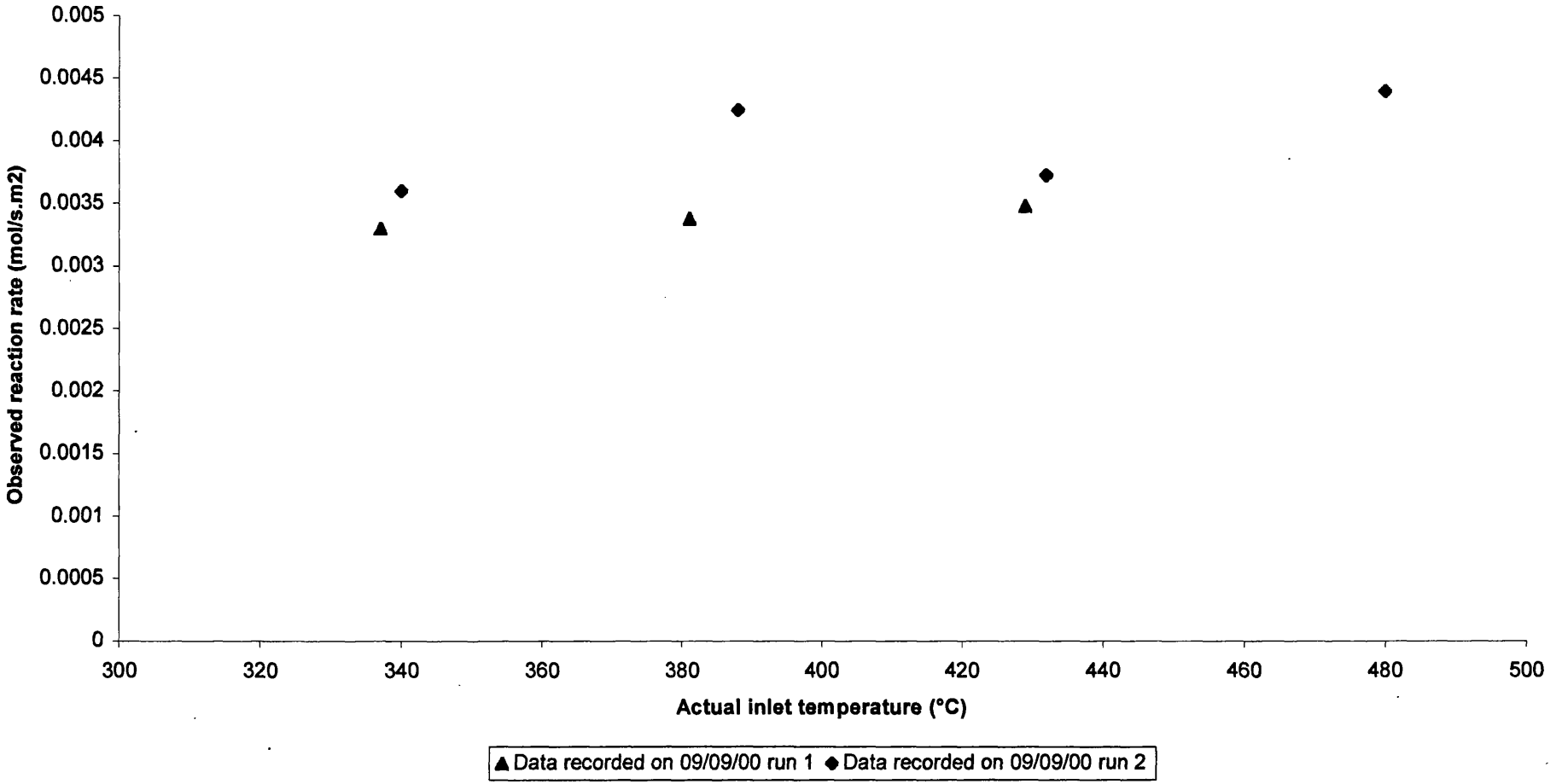
From the raw experimental results, values for the observed reaction rate were calculated as previously described in Chapter 5.

A graph was then plotted of the observed reaction rate against the actual inlet temperature to the reactor for the Degussa catalyst (*Graph 6.25*). This is shown at the end of this section.

From the graph the following conclusions can be drawn:

1. The observed rate of reaction for the Degussa catalyst with 4 g active phase per litre of monolith increases with the reactor inlet temperature. The increase is gradual from a value of $3.5x10^{-3}$ mol/s m^2 at an inlet temperature of 340°C, to a value of $4.5x10^{-3}$ mol/s m^2 at an inlet temperature of 480°C.
2. The results are reproducible as both run 1 and run 2 are in good agreement with each other.

Graph 6.25: Temperature conversion chart for the catalytic combustion of Diesel fuel over Degussa catalyst (4 g Active phase), at constant pressure of 2 bar gauge, constant mass flow and constant Air:Fuel ratio



6.3.2 Pressure Effects

In these experiments the effect of changing the reactor pressure on the catalytic combustion of Diesel fuel was investigated. All other conditions in the test rig were fixed. The Degussa catalysts were assembled into the test rig as described in Chapter 4. The flowrate of air through the rig was fixed at each different pressure to 500 litres/min (Evaluated at 20°C and 1 bar pressure). The Diesel fuel was pumped into the test rig using a metering pump at a fixed rate of 5.6 ml/min, (Chapter 4), (Evaluated at 20°C and 1 bar pressure). The reactor inlet temperature was fixed at 500°C. The pressure in the reactor was varied by adjusting the back-pressure control valve to give pressures varying from 1.5 barg up to 3.5 barg in intervals of 0.5 barg. At each different pressure set point the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in Chapter 3. The experiments were repeated twice and recorded as run 1 and run 2 respectively. The results can be found in Appendix I.

From the raw experimental results, values for the observed reaction rate could be calculated as shown in Chapter 5. Values for the Reynolds number through a channel were also calculated. These results are included with the raw experimental results in Appendix I.

Having calculated the observed reaction rate and Reynolds number through a channel for each pressure studied the following graphs were plotted:

1. The temperature rise across the catalysts against reactor pressure (*Graph 6.26*).
2. The Observed reaction rate against reactor pressure (*Graph 6.27*).
3. The Reynolds number through a channel against reactor pressure (*Graph 6.28*).

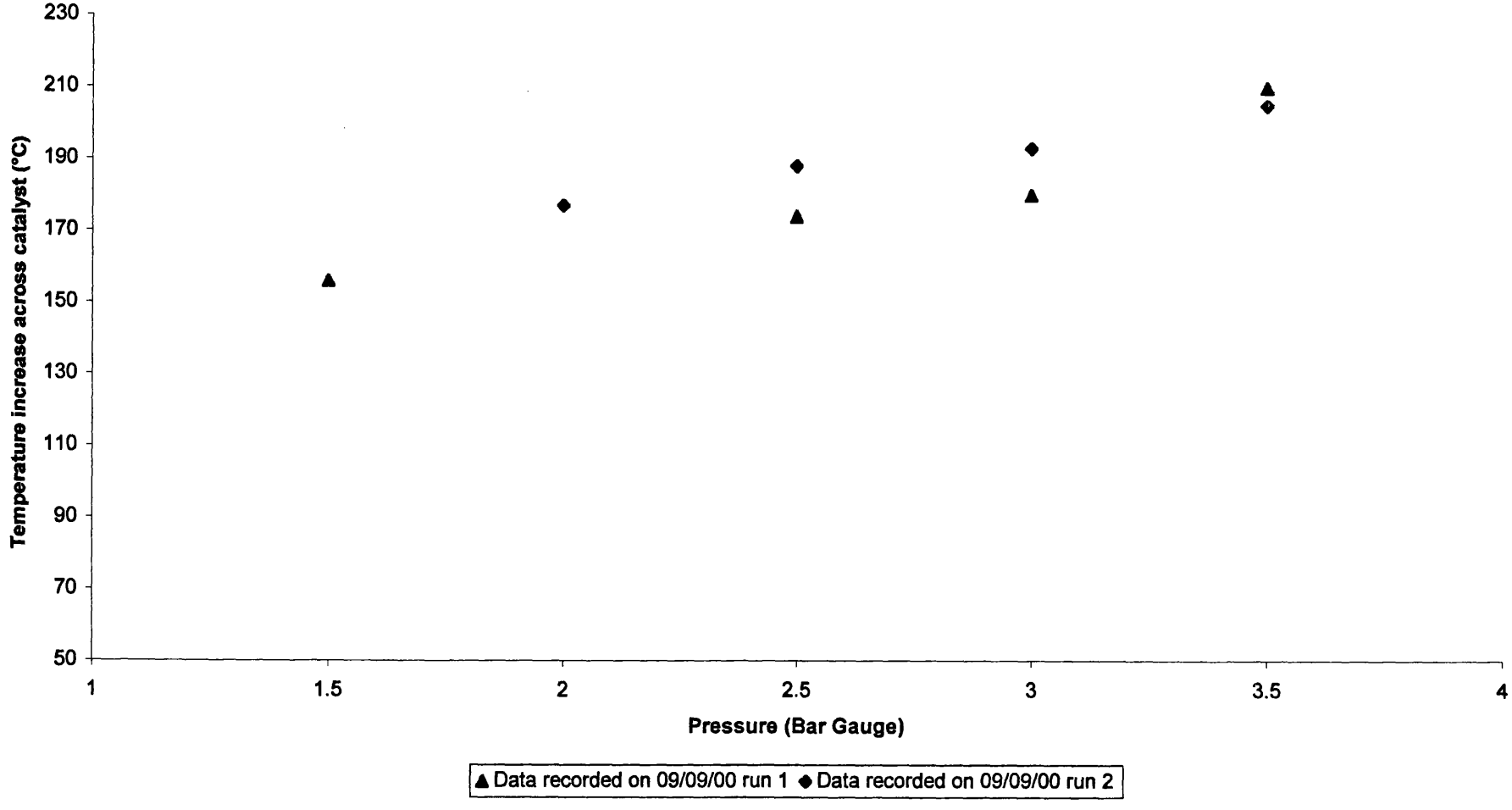
These graphs are all shown at the end of this section.

From these graphs the following conclusions can be drawn:

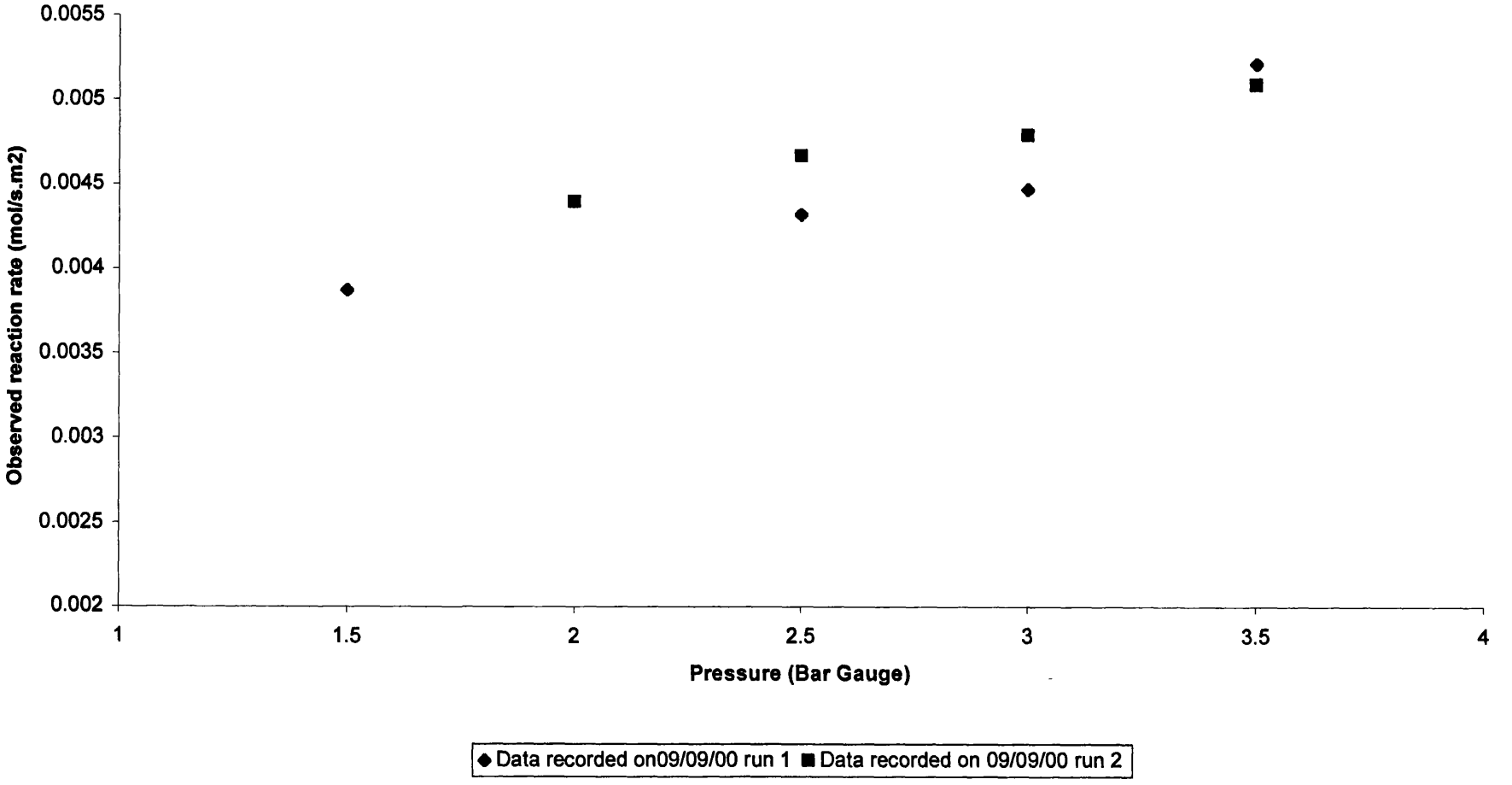
1. The temperature increase across the catalyst increases slightly with pressure. At 1.5 barg the temperature change is approx 150°C, while at 3.5 barg the temperature increase across the catalyst is approx 200°C. This indicates that the catalytic combustion of Diesel fuel using the Degussa catalyst shows a slight dependence on pressure.
2. The observed rate of reaction increases slightly with an increase in pressure. At 1.5 barg the observed rate of reaction is approx $3.9x10^{-3}$ mol/s.m^2, which increases to approx $5.1x10^{-3}$ mol/s m^2 at 3.5 barg. The increase indicates that the catalytic combustion of Diesel fuel over the Degussa catalysts is slightly dependent on pressure.
3. The Reynolds number through a channel shows minor fluctuations with pressure, but is approx constant at 2500 over the range of pressures studied. This indicates Transitional flow through the channels, and that the observed changes in the rate of reaction noticed with increasing pressure is not a result of changes in the Reynolds number.

All the results are repeatable as both run 1 and run 2 are in close agreement.

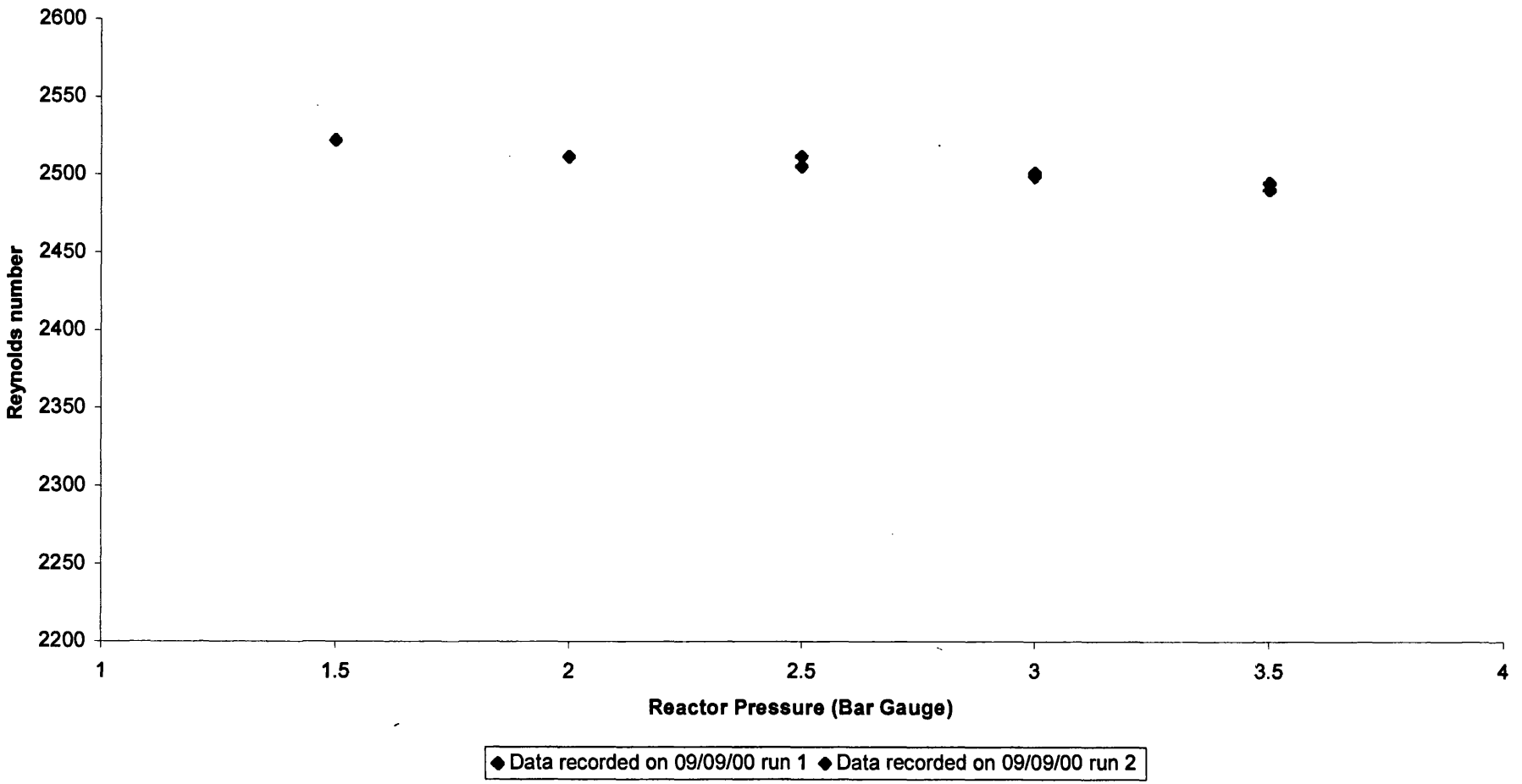
Graph 6.26: Effect of pressure on the catalytic combustion of Diesel over Degussa catalyst (4g Active phase), at a constant throughput and a constant inlet setpoint temperature of 500°C



Graph 6.27: Effect of pressure on the catalytic combustion of Diesel over Deguusa catalyst (4g Active phase), at a constant throughput and a constant inlet setpoint temperature of 500°C



Graph 6.28: Reynolds number against reactor pressure for the catalytic combustion of diesel fuel over Degussa catalyst (4g active phase), at constant throughput and constant inlet setpoint temperature of 500°C



Chapter 7: Discussion and overall conclusions.

7.1 Control experiments.

7.1.1 Experiments with blank monoliths

Experiments were performed using blank monoliths of fixed dimensions, with only a washcoat covering to establish whether washcoated monoliths show any catalytic activity for the combustion of both diesel fuel and unleaded petrol. All monoliths had an initial gamma alumina washcoat layer of approx 112 g alumina per litre of monolith, which were calcined to 500°C. Full details on the production of the catalysts can be found in the Chapter 4.

In these experiments the effect of changing the catalyst inlet temperature on the catalytic combustion of diesel fuel and unleaded petrol was investigated. All other conditions in the test rig were fixed. The blank catalysts were assembled into the test rig as described in the Chapter 3. The flowrate of air through the rig was fixed at 500 litres/min (Evaluated at 20°C and 1 bar pressure). The Diesel Fuel was pumped into the test rig using a metering pump at a fixed rate of 5.6 ml/min, (Chapter 4), (Evaluated at 20°C and 1 bar pressure), and the unleaded petrol was pumped using the same equipment at a rate of 6.1 ml/min, (Chapter 4), (Evaluated at 20°C and 1 bar pressure). The reactor pressure was fixed at 2 barg using a back-pressure control valve. The catalyst inlet temperature was varied by altering the electric air heater set point from 350°C to 500°C in increments of 50°C. At each different temperature set point the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in the Chapter 3. The experimental results for both diesel fuel and unleaded petrol can be found in Appendix J.

From the raw experimental results, values for the observed reaction rate were calculated as shown previously in Chapter 5. The calculation was performed for every inlet set point temperature studied, and for both diesel fuel and unleaded petrol. The results are included with the raw experimental results in Appendix J.

From the results it can be seen that the blank washcoated monoliths show no catalytic activity for the combustion of either diesel fuel or unleaded petrol.

7.1.2 Combustion of methane

Experiments were performed using the Degussa (4 g active phase per litre of monolith), platinum (8 g active phase per litre of monolith) and Perovskite (24 g active phase per litre of monolith) catalysts to investigate their performance for the combustion of methane. All monoliths had an initial gamma alumina washcoat layer of approx 112 g alumina per litre of monolith, which were calcined to 500°C before the active phases were added as described in the full details on the production of the catalysts found in the Chapter 4.

In these experiments the effect of changing the catalyst inlet temperature on the catalytic combustion of methane was investigated. All other conditions in the test rig were fixed. The blank catalysts were assembled into the test rig as described in the Chapter 3. The flowrate of air through the rig was fixed at 500 litres/min (Evaluated at 20°C and 1 bar pressure). The methane was supplied into the test rig using a calibrated mass flow controller at a fixed rate of 9 litres/min, (Chapter 4), (Evaluated at 20°C and 1 bar pressure). The reactor pressure was fixed at 2 barg using a back-pressure control valve. The catalyst inlet temperature was varied by altering the electric air heater set point from 350°C to 500°C in increments of 50°C. At each different temperature set point the catalyst wall, outlet and actual inlet temperatures were recorded along with the total hydrocarbon content of the inlet and outlet streams. Full details on the experimental apparatus and procedures are shown in the Chapter 3. The experimental results for all three of the different catalysts can be found in Appendix K.

From the raw experimental results, values for the observed reaction rate were calculated as shown previously in Chapter 5. The calculation was performed for every inlet set point temperature studied, and for all of the different catalysts. The results are included with the raw experimental results in Appendix K.

From the results it can be seen that none of the catalysts showed any catalytic activity for the combustion of methane over the range of inlet temperatures studied.

It can therefore also be concluded that the catalysts with lower amounts of active phase (platinum catalyst with 4 g active phase per litre of monolith, and the perovskite catalyst with 8 g active phase per litre of monolith) would also have shown no catalytic activity for methane under the range of inlet temperatures studied.

7.2 Comparison of the catalysts for the combustion of liquid fuels.

From the experimental results described in Chapters 5 and 6 some comparisons between the different catalysts can be made.

7.2.1 Comparison of performance for the combustion of diesel fuel

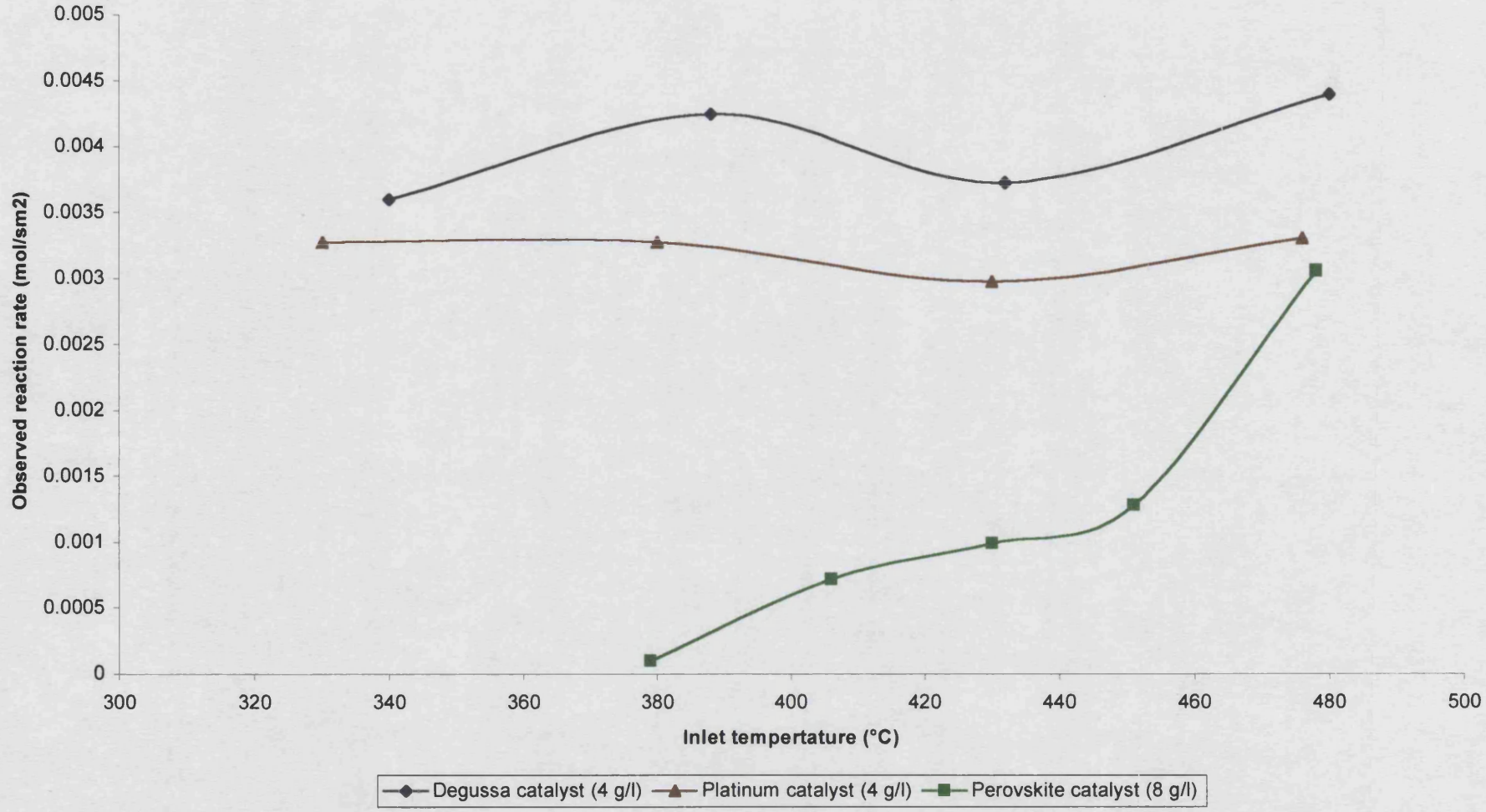
A comparison of the performance of the Degussa catalyst (4 g active phase per litre of monolith), the platinum catalyst (4 g active phase per litre of monolith) and the perovskite catalyst (8 g active phase per litre of monolith) for the catalytic combustion of diesel fuel was undertaken. This was achieved by taking the observed reaction rate results obtained by varying the inlet temperature set point for each of the catalysts (Chapter 6) and plotting the resulting curves on the same axis. *Graph 7.1* (shown at the end of this section) details this comparison.

It can be seen from this comparison that the Degussa catalyst shows the highest activity for the catalytic combustion of diesel fuel over the entire range of inlet temperatures studied. The platinum catalyst shows slightly lower activity than the Degussa catalyst but a greater activity than the perovskite catalyst, which shows the lowest activity of all of the catalysts, apart from at very high inlet temperatures when its activity becomes comparable to the platinum catalyst.

As both the Degussa and Platinum catalysts contained 4 g of platinum per litre of monolith they would be expected to exhibit the same activity for the catalytic combustion of diesel fuel, however, the Degussa catalyst has been shown to have a greater activity across the range of inlet temperatures studied. This could be

explained by differences in the catalyst production methods and by differences in the catalysts physical characteristics e.g. BET surface area measurements. These characteristics will be discussed later in this Chapter.

Graph 7.1: Comparison of the different catalysts for the catalytic combustion of diesel fuel



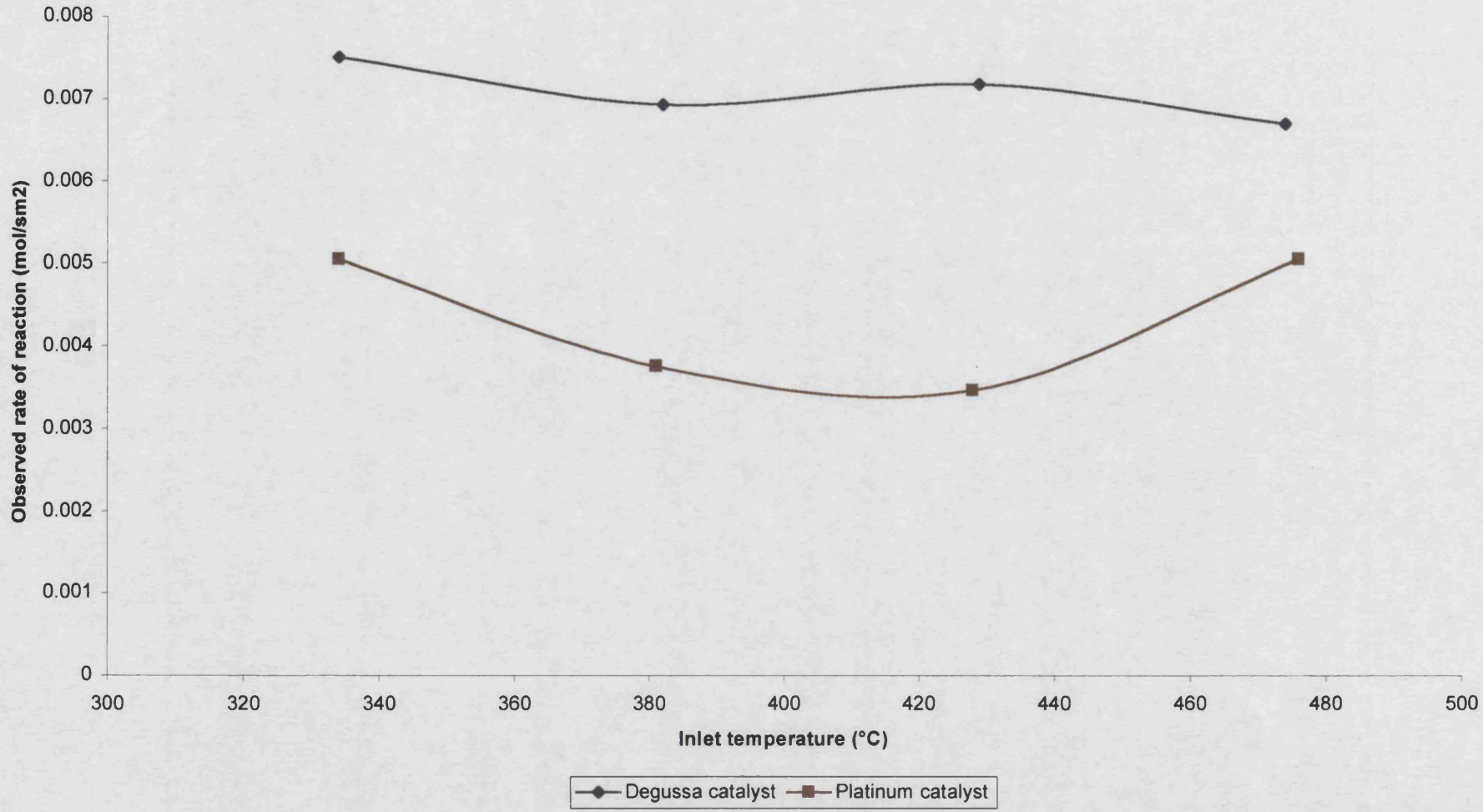
7.2.2 Comparison of performance for the combustion of unleaded petrol

A comparison of the performance of the Degussa catalyst (4 g active phase per litre of monolith), and the platinum catalyst (4 g active phase per litre of monolith) for the catalytic combustion of unleaded petrol was also undertaken. This was achieved by taking the observed reaction rate results obtained by varying the inlet temperature set point for each of the catalysts (Chapter 5) and plotting the resulting curves on the same axis. *Graph 7.2* (shown at the end of this section) details this comparison.

It can be seen from this comparison that the Degussa catalyst shows the highest activity for the catalytic combustion of diesel fuel over the entire range of inlet temperatures studied. Both of the perovskite catalysts exhibited no catalytic activity for unleaded petrol and were therefore omitted from this comparison.

As both the Degussa and Platinum catalysts contained 4 g of platinum per litre of monolith they would be expected to exhibit the same activity for the catalytic combustion of unleaded petrol, however, the Degussa catalyst has been shown to have a greater activity across the range of inlet temperatures studied. This could be explained by differences in the catalyst production methods and by differences in the catalysts physical characteristics e.g. BET surface area measurements. These characteristics will be discussed later in this Chapter.

Graph 7.2: Comparison of different catalysts for the catalytic combustion of unleaded petrol



7.2.3 Comparison of performance of the Degussa catalyst for the combustion of Unleaded petrol and diesel fuel

A comparison of the performance of the Degussa catalyst (4 g active phase per litre of monolith) for the catalytic combustion of unleaded petrol and diesel fuel was undertaken. This was achieved by taking the observed reaction rate results obtained by varying the inlet temperature set point for each of the two fuels (Chapter 5 & 6) and plotting the resulting curves on the same axis. *Graph 7.3* (shown at the end of this section) details this comparison.

It can be seen from this comparison that the Degussa catalyst shows the highest activity for the catalytic combustion of unleaded petrol over the entire range of inlet temperatures studied.

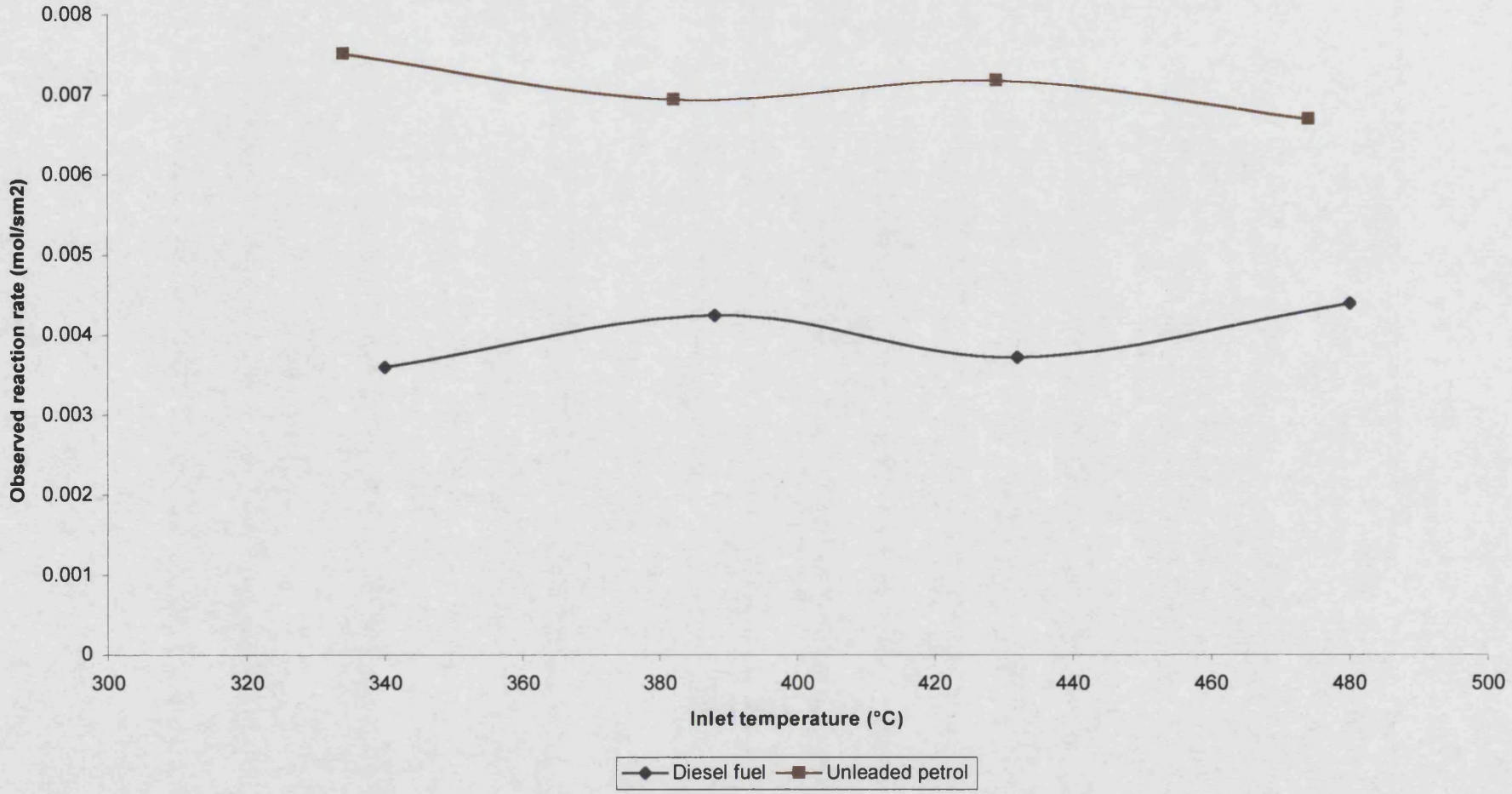
7.2.4 Comparison of performance of the platinum catalyst for the combustion of Unleaded petrol and diesel fuel

A comparison of the performance of the platinum catalyst (4 g active phase per litre of monolith) for the catalytic combustion of unleaded petrol and diesel fuel was undertaken. This was achieved by taking the observed reaction rate results obtained by varying the inlet temperature set point for each of the two fuels (Chapter 5 & 6) and plotting the resulting curves on the same axis. *Graph 7.4* (shown at the end of this section) details this comparison.

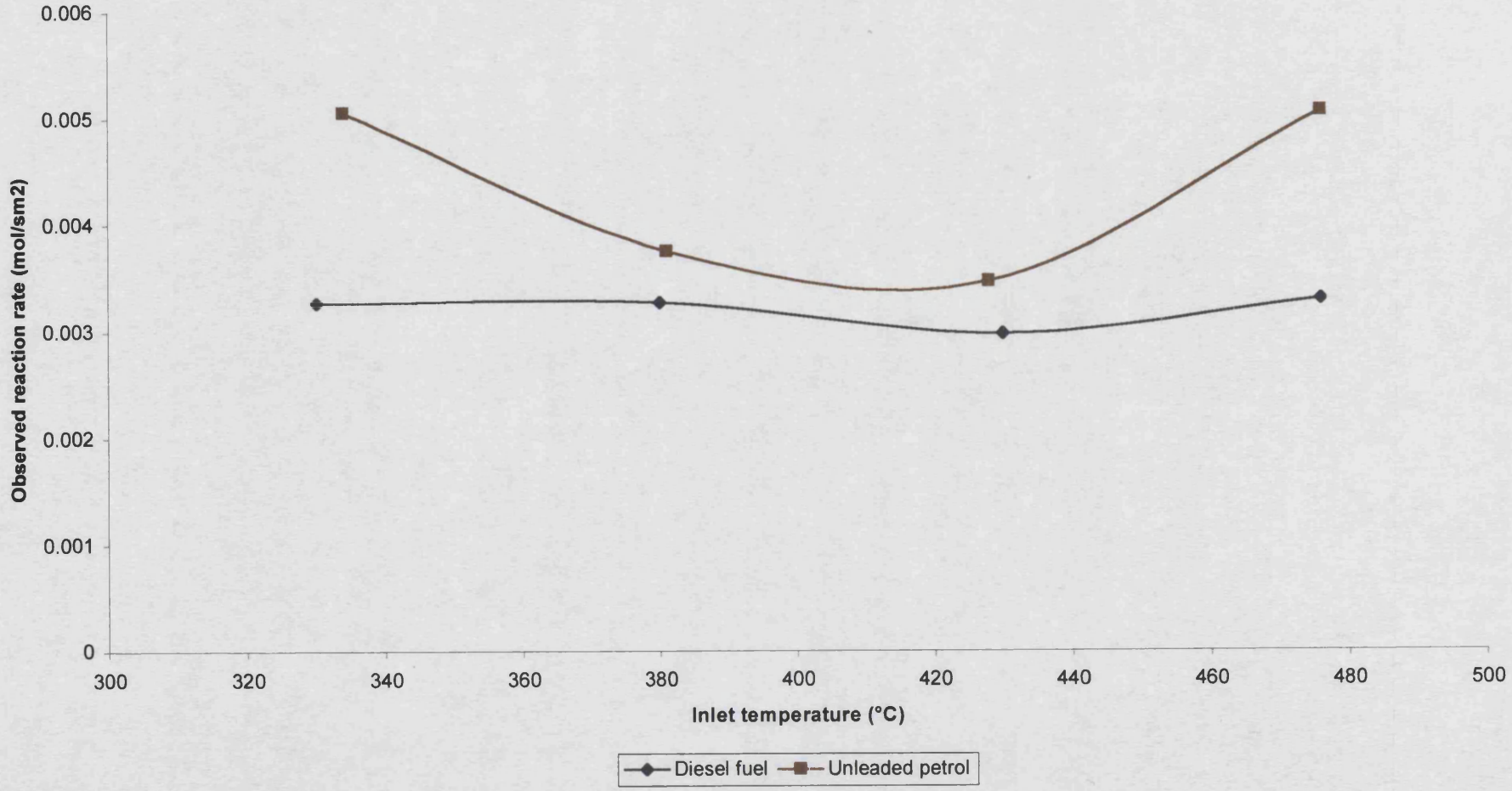
It can be seen from this comparison that the platinum catalyst shows the highest activity for the catalytic combustion of unleaded petrol over the entire range of inlet temperatures studied.

A comparison of the perovskite for the catalytic combustion of unleaded petrol and diesel fuel was not performed because the perovskite catalyst showed no catalytic activity for the combustion of unleaded petrol. Methane was not included in the comparisons as none of the catalysts showed any catalytic activity for this fuel over the range of inlet temperatures studied.

Graph 7.3: Comparison of the degussa catalyst (4 g active phase per litre of monolith) for the catalytic combustion of diesel fuel and unleaded petrol



Graph 7.4: Comparison of the platinum catalyst (4 g platinum per litre of monolith) for the catalytic combustion of diesel fuel and unleaded petrol



7.3 Comparison of the observed reaction rates obtained by temperature measurements and by analyser readings.

The observed reaction rates for all the catalysts have been calculated in the results described in Chapters 5 & 6 by utilising the temperature difference across the catalysts and comparing to the adiabatic temperature rise associated with 100% conversion. To check the validity of this calculation, comparisons can be made for each catalyst and both the liquid fuels studied by calculating the observed reaction rate from the total hydrocarbon reading taken at each experiment and comparing to the observed reaction rate obtained using temperature differences. Total hydrocarbon readings were taken during each experiment, sampling the inlet stream to the catalysts and the outlet stream from the catalysts. These values have been included in the appropriate experimental results in the Appendices. The following example calculation illustrates how the observed reaction rate can be calculated from the total hydrocarbon analyser readings. It is based on the platinum catalyst containing 4 g active phase per litre of monolith for the combustion of diesel fuel studying the affect of changing the inlet temperature at an inlet set point temperature of 400°C. The data was recorded on the 7th September 2000 Run 1 and can be located in Appendix G.

Inlet total hydrocarbon reading = 2850 ppm
Outlet total hydrocarbon reading = 1460 ppm

$$\Rightarrow \quad \text{Fractional conversion} = \frac{2850-1460}{2850} \times 100 = 48.8\%$$

Molar flowrate of diesel into reactor = 3.92×10^{-4} mol/s (Calculated as shown in Chapters 5 & 6).

$$\Rightarrow \quad \text{Moles of diesel combusted} = 0.488 \times 3.92 \times 10^{-4} = 1.91 \times 10^{-4} \text{ mol/s}$$

Geometric surface area of catalyst = 5.25×10^{-2} m^2 (Calculated in Chapter 5)

$$\Rightarrow \quad \text{Observed reaction rate} = \frac{1.91x10^{-4}}{5.25x10^{-2}} = 3.48x10^{-3} \text{ mol/s.m}^2$$

This calculation was performed for every experimental reading taken and the results have been included in all the appropriate Appendices.
The following graphs were then plotted showing the observed reaction rate calculated based on temperature measurements against the observed reaction rate calculated from total hydrocarbon analyser readings (the graphs are included at the end of this section):

Graph 7.5: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of diesel fuel over the platinum catalyst (4 g active phase per litre of monolith)

Graph 7.6: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of unleaded petrol over the platinum catalyst (4 g active phase per litre of monolith)

Graph 7.7: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of diesel fuel over the platinum catalyst (8 g active phase per litre of monolith)

Graph 7.8: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of Unleaded petrol over the platinum catalyst (8 g active phase per litre of monolith)

Graph 7.9: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of diesel fuel over the Degussa catalyst (4 g active phase per litre of monolith)

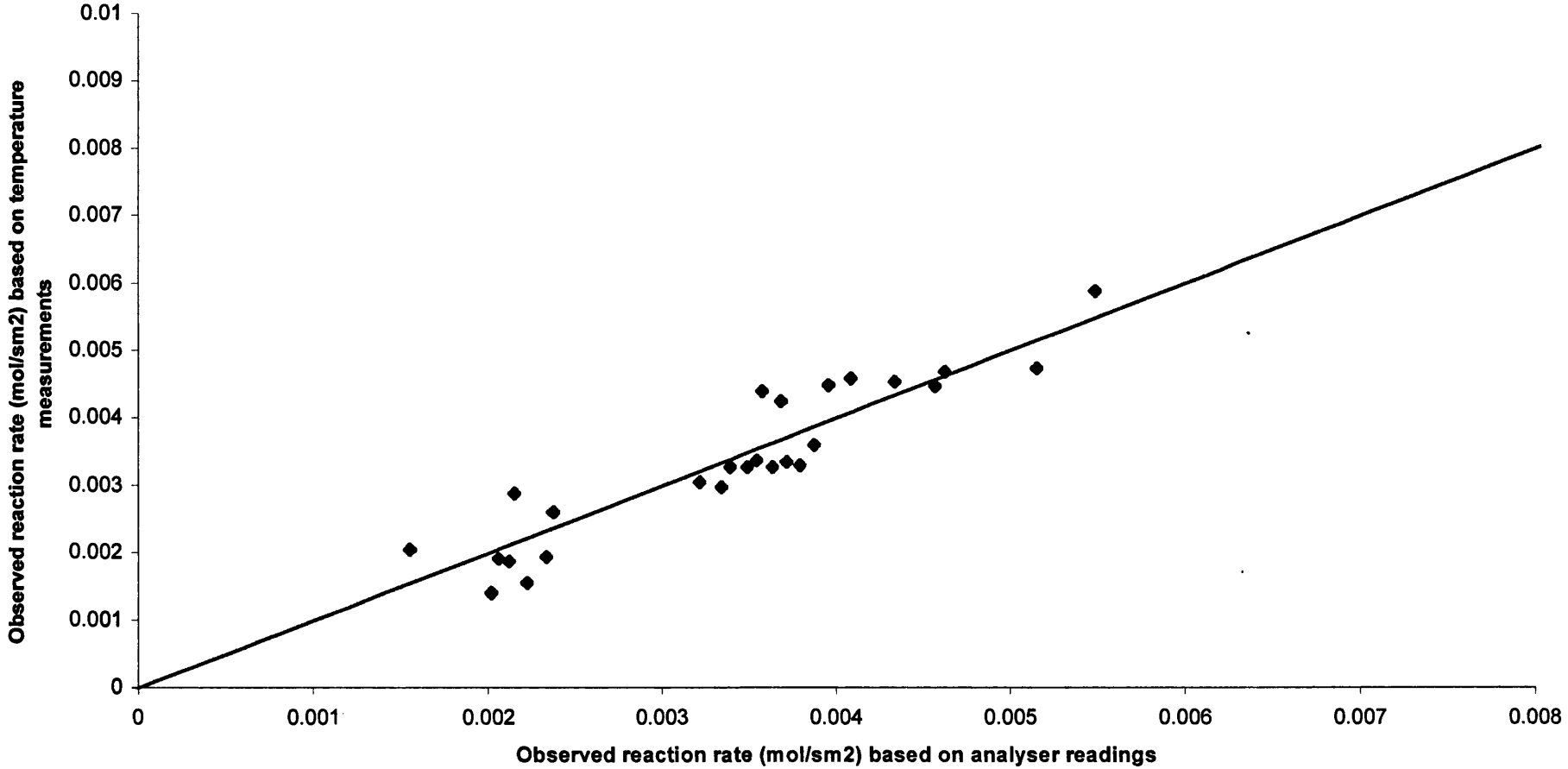
Graph 7.10: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of Unleaded petrol over the Degussa catalyst (4 g active phase per litre of monolith)

Graph 7.11: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of diesel fuel over the perovskite catalyst (8 g active phase per litre of monolith)

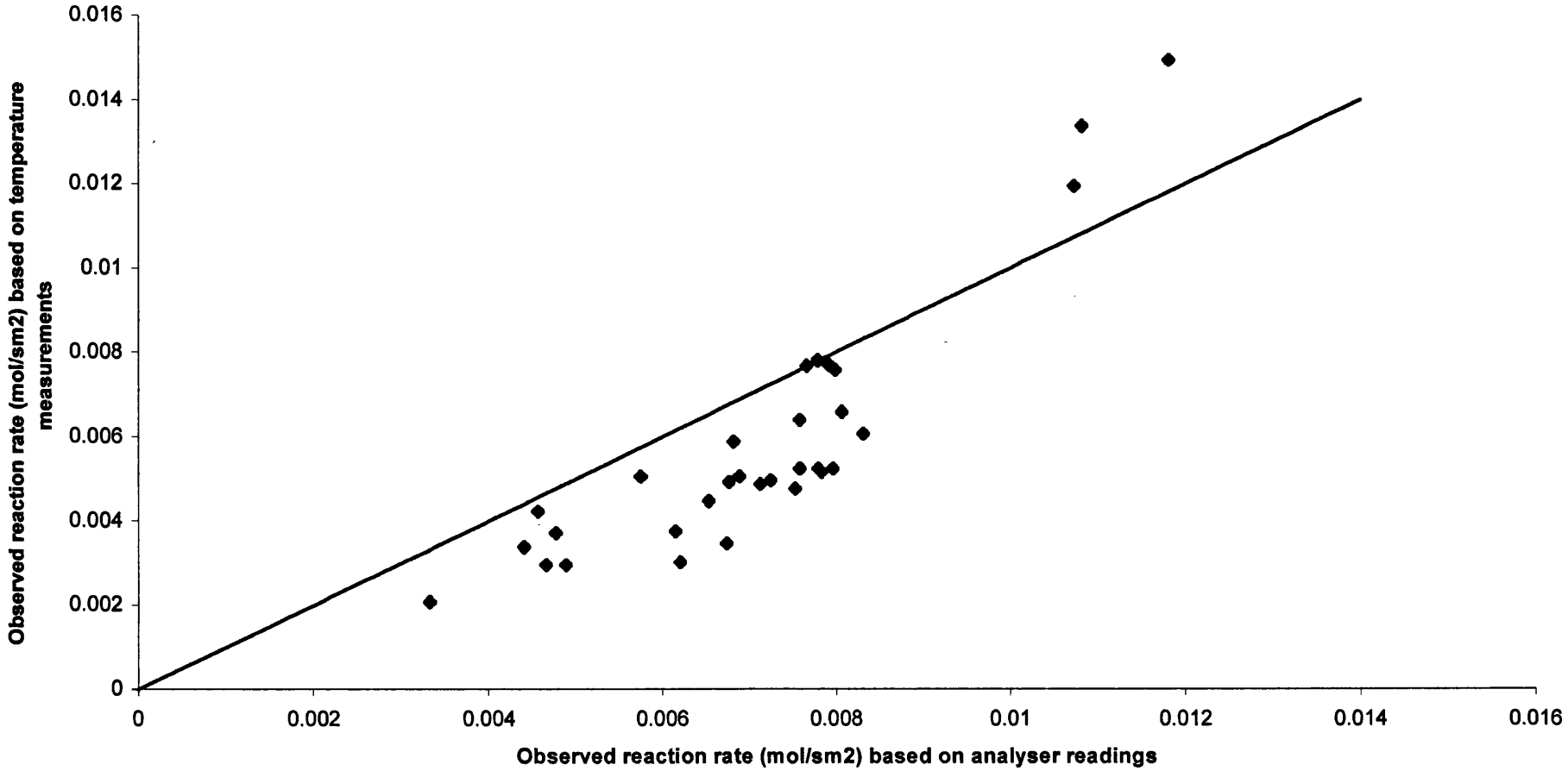
Graph 7.12: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of diesel fuel over the perovskite catalyst (24 g active phase per litre of monolith)

Studying all of the graphs it can be seen that the data points all lie near or on the y=x line hence the observed reaction rate calculated based on temperature measurements and the observed reaction rate calculated from total hydrocarbon analyser readings are all approximately similar. This implies that the use of temperature measurements in the calculation of the observed reaction rates can be justified.

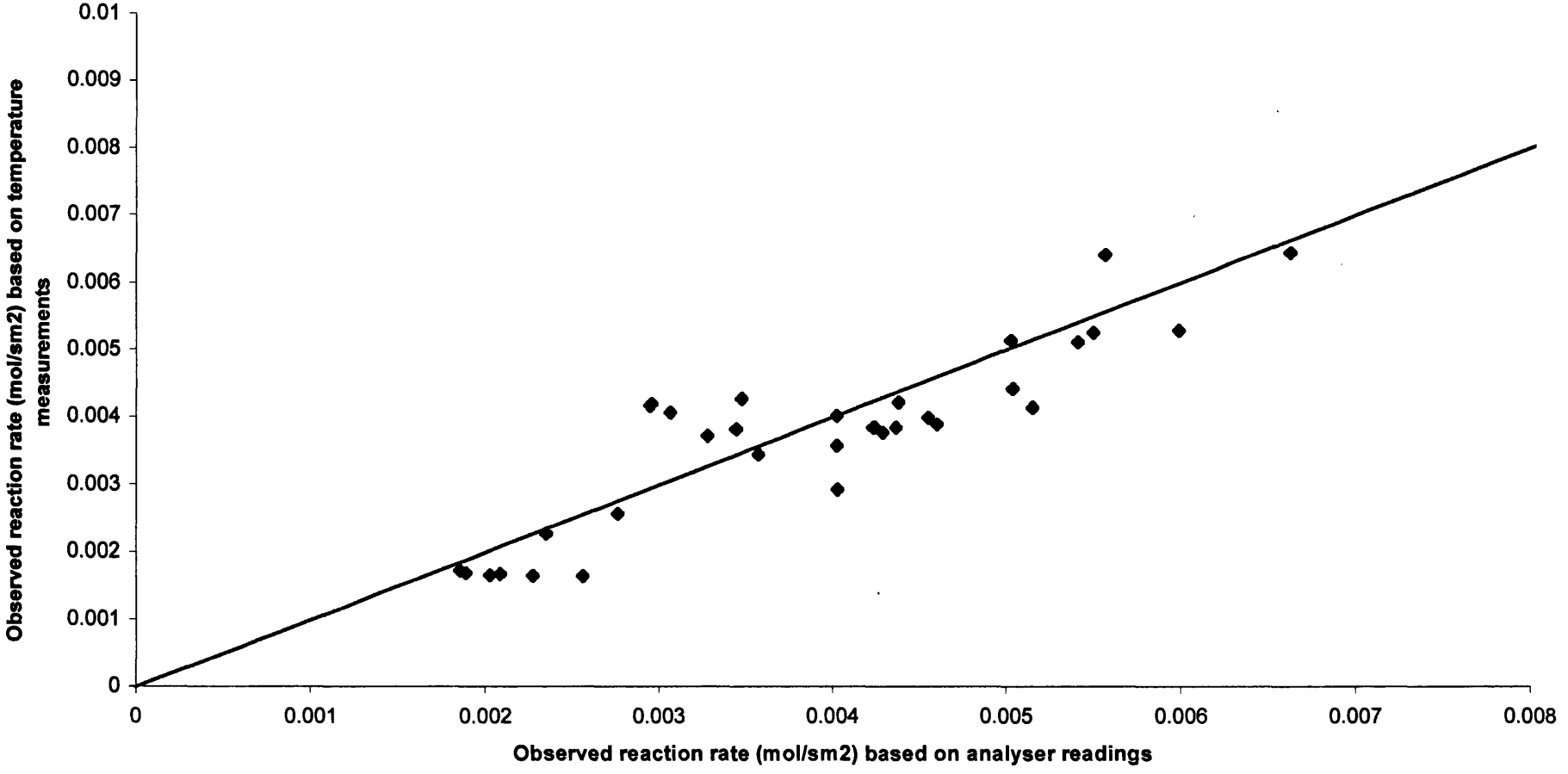
Graph 7.5: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of diesel fuel over platinum catalyst (4 g active phase per litre of monolith)



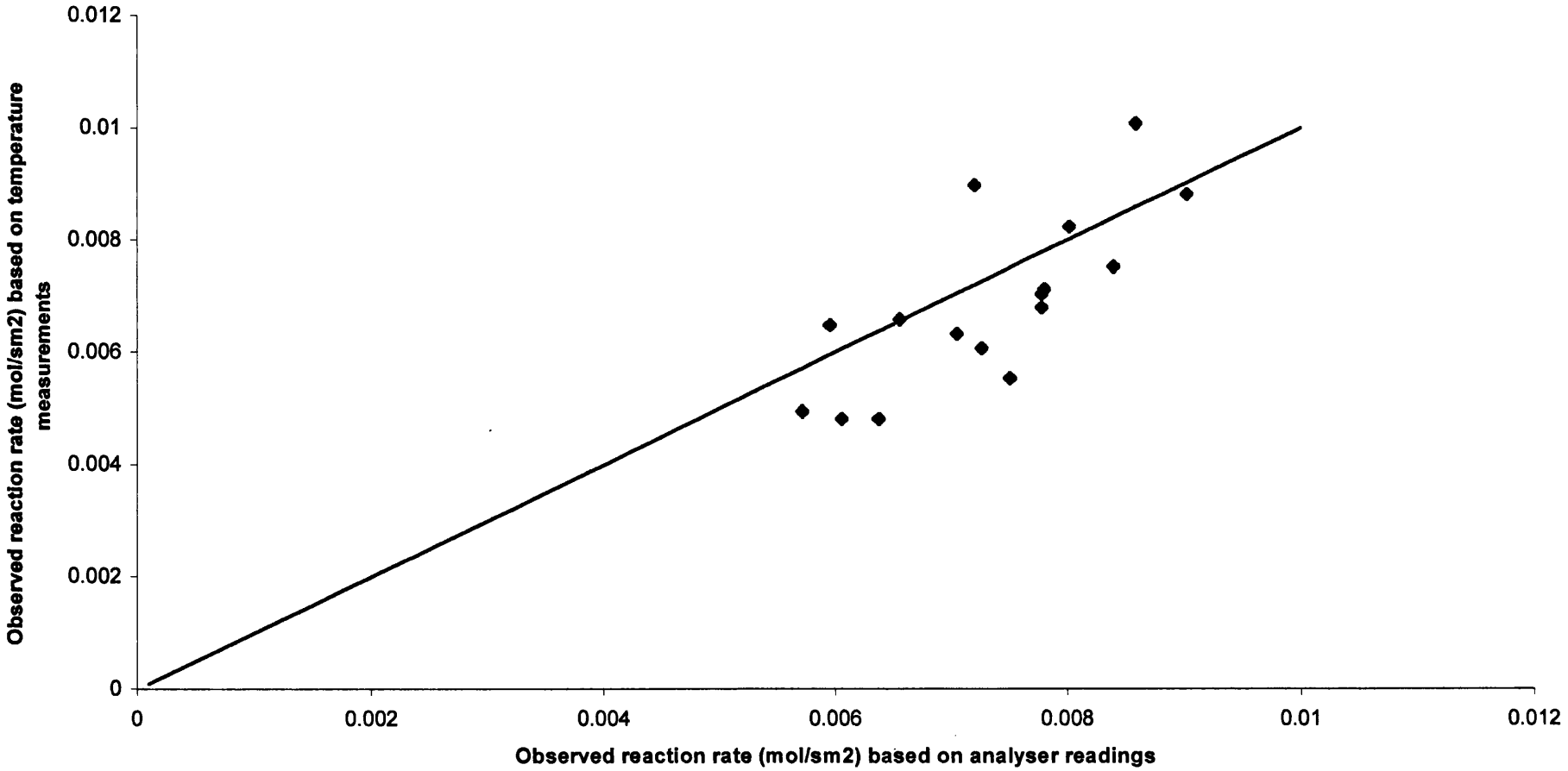
Graph 7.6: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of unleaded petrol over platinum catalyst (4g platinum per litre of monolith)



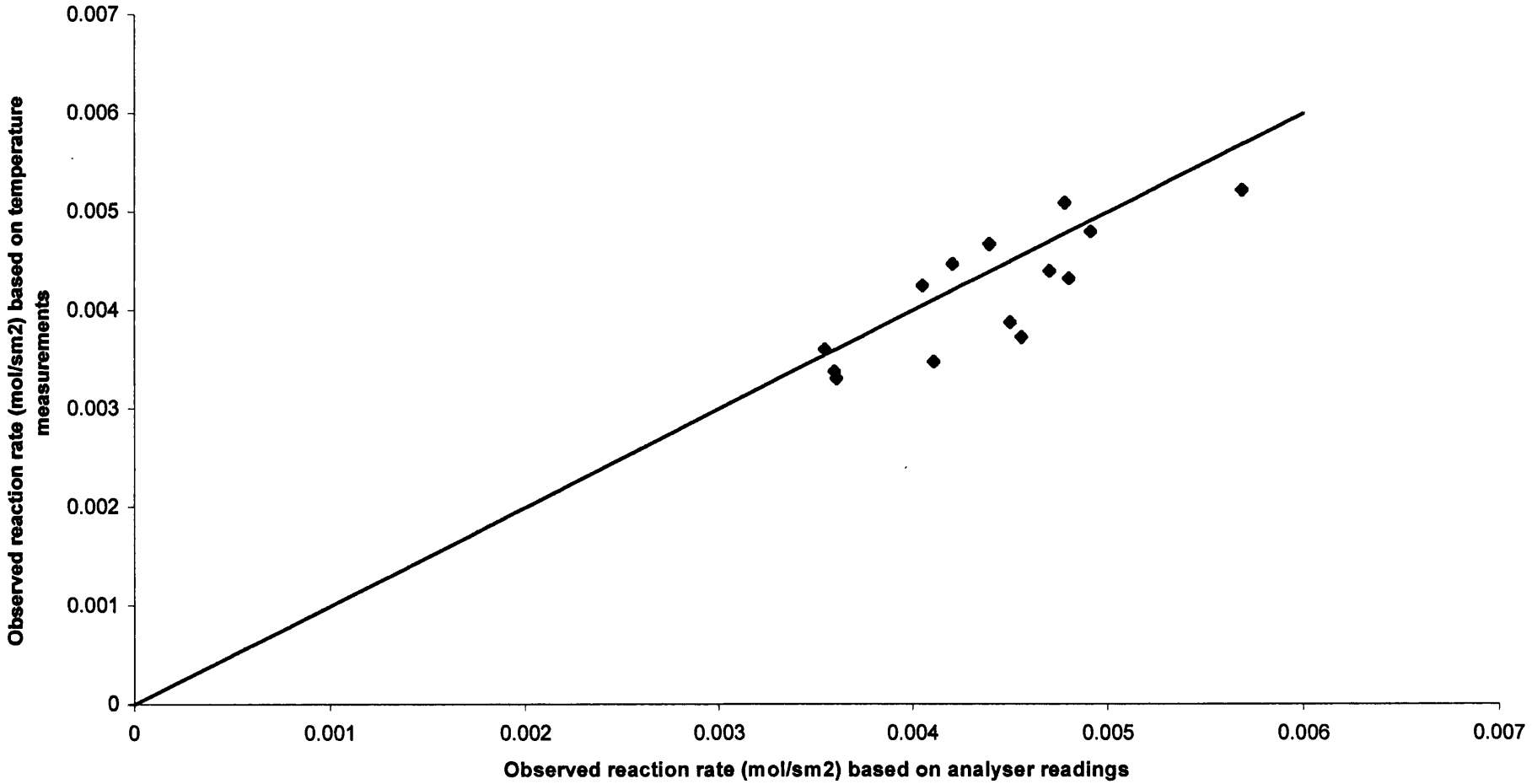
Graph 7.7: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of diesel fuel over platinum catalyst (8 g active phase per litre of monolith)



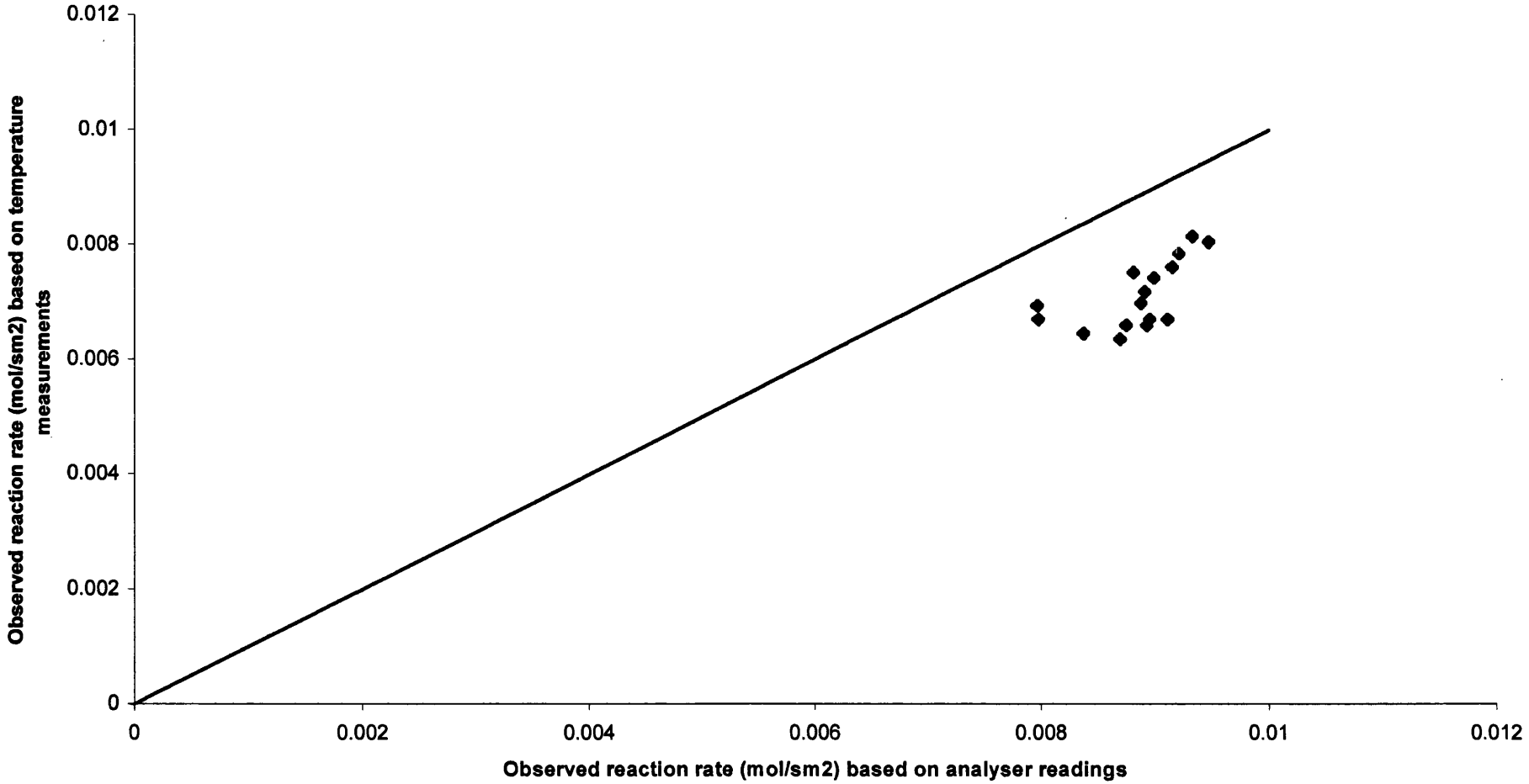
Graph 7.8: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of unleaded petrol over platinum catalyst (8g platinum per litre of monolith)



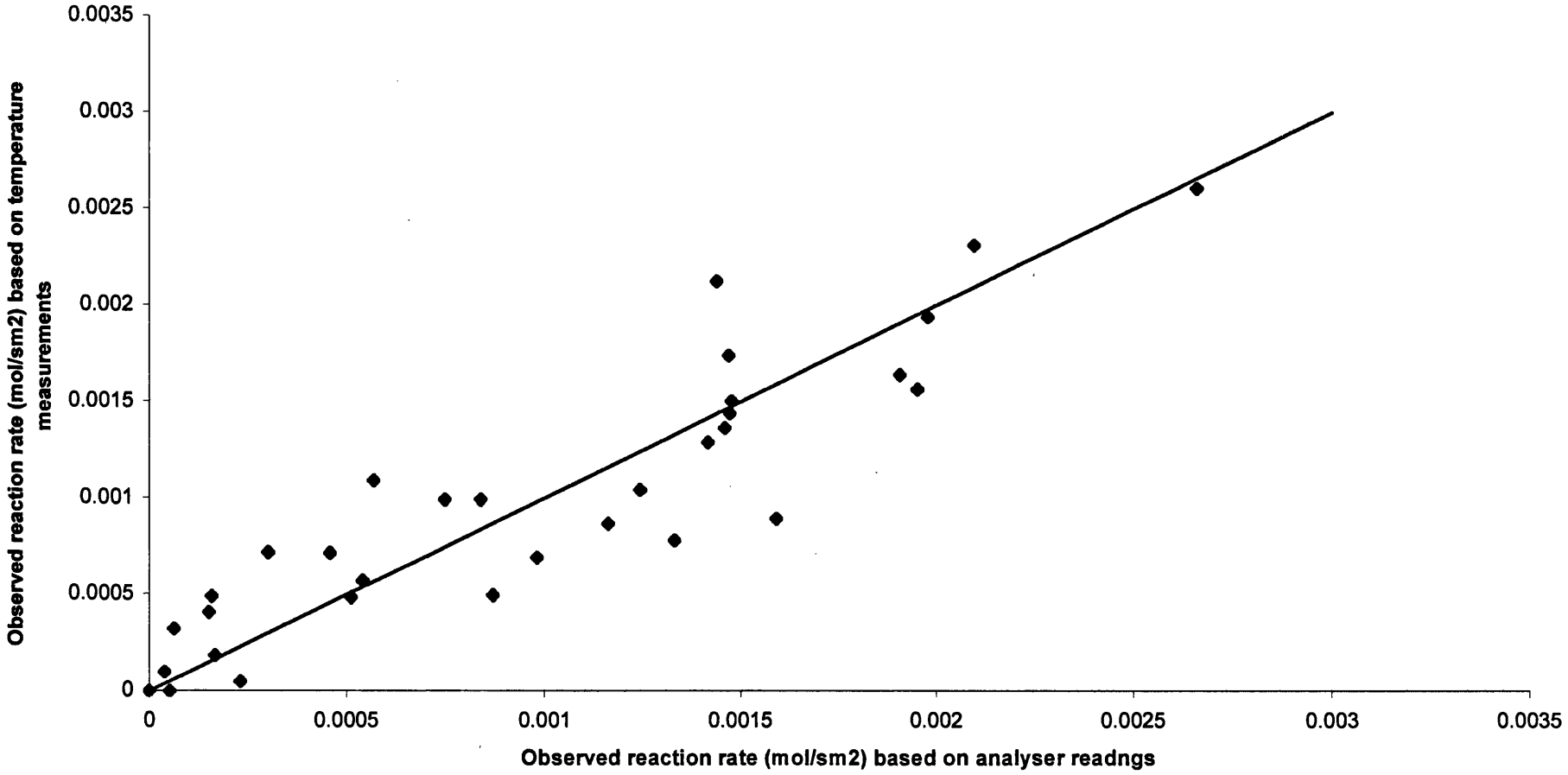
Graph 7.9: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of diesel fuel over Degussa catalyst



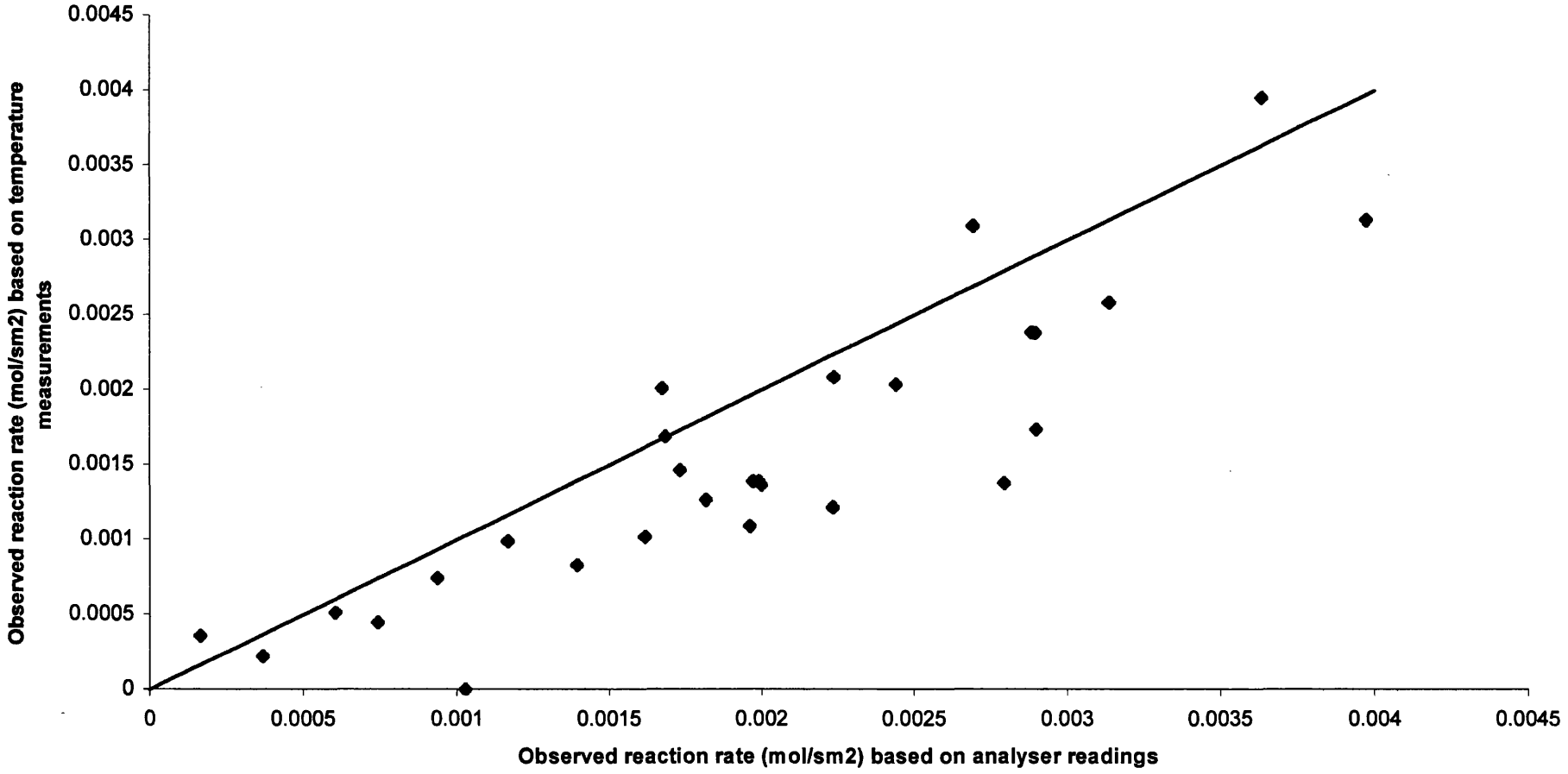
Graph 7.10: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of unleaded petrol over Degussa catalyst



Graph 7.11: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of diesel fuel over perovskite catalyst (8 g active phase per litre of monolith)



Graph 7.12: Comparison of observed reaction rate calculated by temperature measurements and analyser readings for the catalytic combustion of diesel fuel over perovskite catalyst (24 g active phase per litre of monolith)

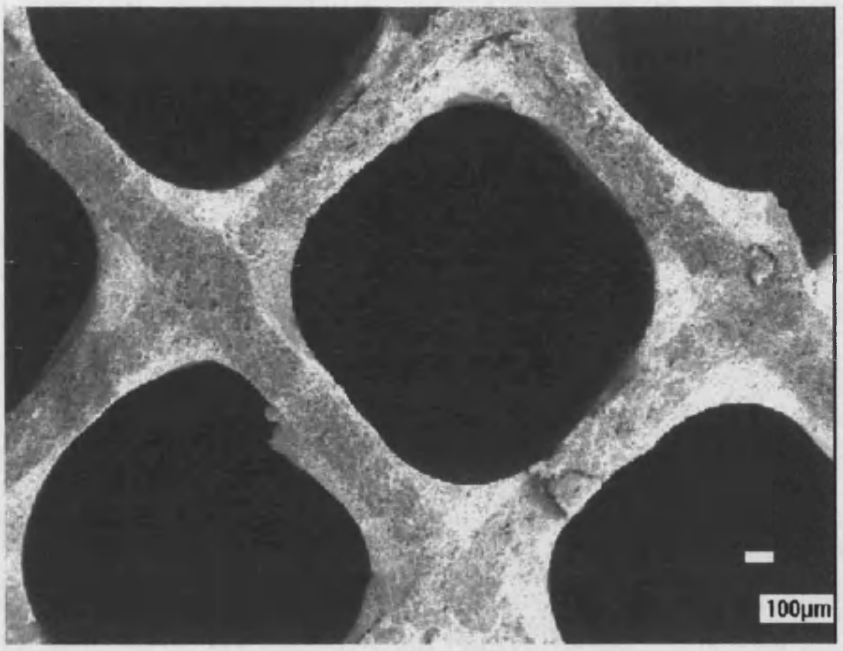


7.4 Catalyst Characteristic results

7.4.1 SEM analysis

SEM images were obtained for each of the catalysts studied. The images can be used to obtain accurate dimensions of a single cell which affects the value of the total geometric surface area used in the calculation for the observed reaction rate. The catalyst samples used for this analysis were uneven in shape and therefore the electron microscope camera did not see a truly "straight" sample. The images are therefore offset from the horizontal and can only be used to give an approximation of the actual cell dimensions. An approximate "error" in the geometric surface area used to in the calculation of the observed reaction rate based on the assumption that the cells are 1mm by 1mm can be calculated from these images, however, it should be noted that the actual dimensions could not be ascertained. This approximate "error" to the observed reaction rates for each catalyst is shown underneath the SEM image for that catalyst

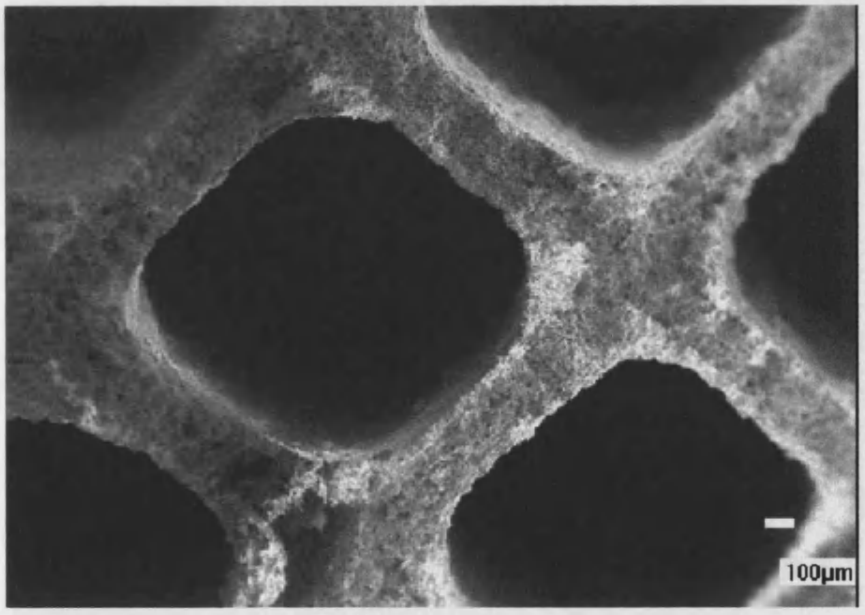
The Degussa catalyst



Approximate internal dimension of cell = 1.05mm x 1.05 mm

⇒ Approximate "error" in observed reaction rate = -5%

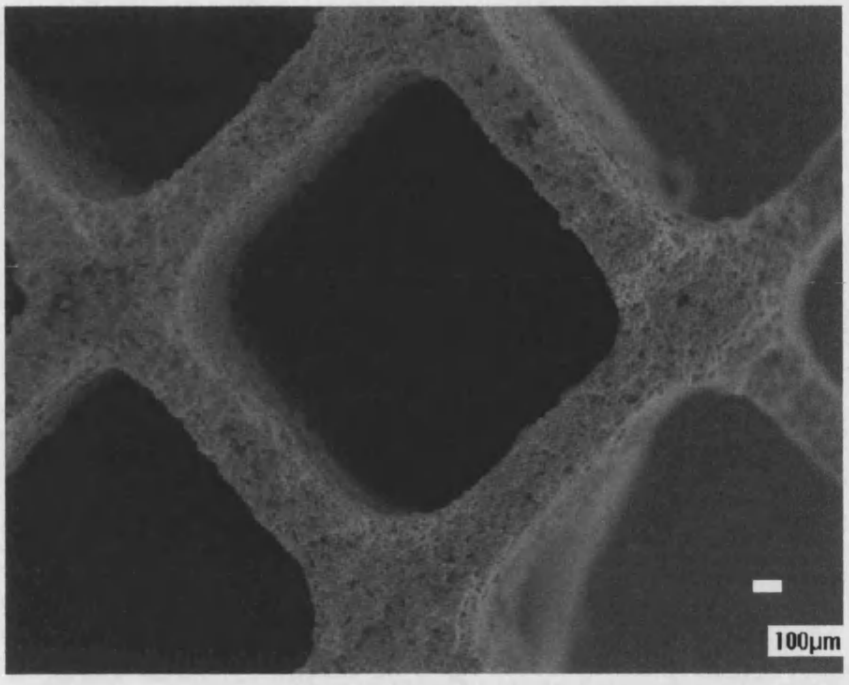
The Platinum catalyst (4 g active phase per litre of monolith)



Approximate internal dimension of cell = 1.00 mm x 1.00 mm

⇒ Approximate "error" in observed reaction rate = 0%

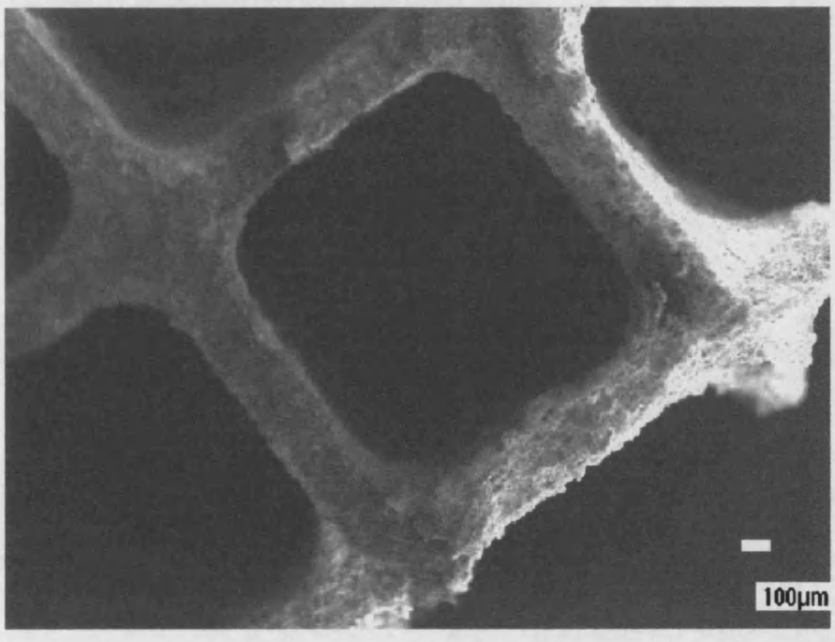
The Platinum catalyst (8 g active phase per litre of monolith)



Approximate internal dimension of cell = 1.08 mm x 1.08 mm

⇒ Approximate "error" in observed reaction rate = -8%

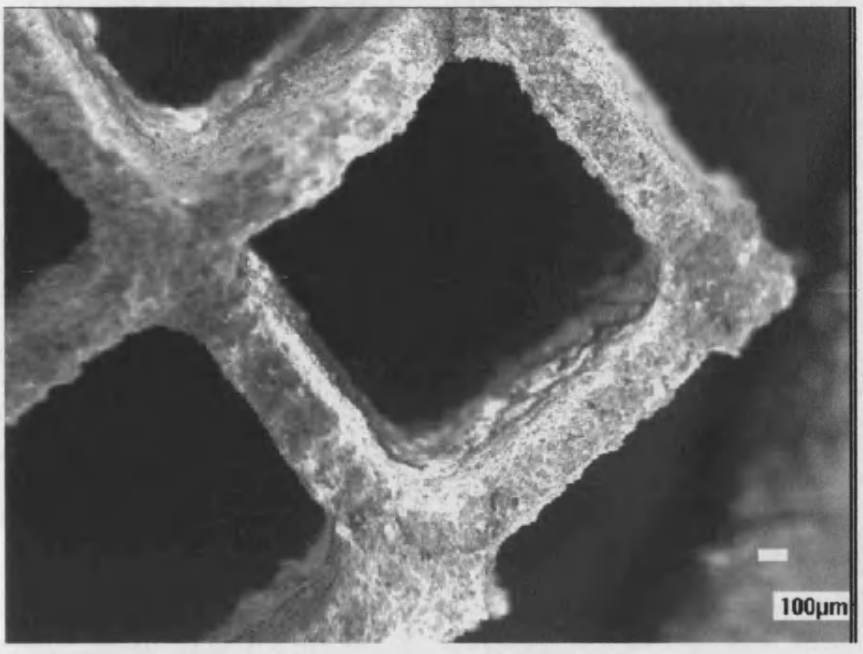
The perovskite catalyst (8 g active phase per litre of monolith)



Approximate internal dimension of cell = 1.03 mm x 1.03 mm

⇒ Approximate "error" in observed reaction rate = -3%

The perovskite catalyst (24 g active phase per litre of monolith)



Approximate internal dimension of cell = 1.05 mm x 1.05 mm

⇒ Approximate "error" in observed reaction rate = -5%

As can be seen from the SEM data, the approximate "error" in the observed reaction rate is approximately zero for catalysts with 4 g active phase per litre of monolith, and increases with increased amount of active phase.

7.4.2 BET analysis

BET surface area results were obtained for each of the catalysts studied. The results are summarised in *Table 7.1* below

Catalyst	BET surface area (m^2/g)
Degussa (4 g active phase per litre of monolith)	49.7163
Platinum (4 g active phase per litre of monolith)	34.2075
Platinum (8 g active phase per litre of monolith)	23.6822
Perovskite (8 g active phase per litre of monolith)	26.666
Perovskite (24 g active phase per litre of monolith)	29.1909

The Degussa catalyst has the highest surface area result. This catalyst also showed the greatest catalytic activity for both diesel fuel and unleaded petrol. This could be because the increased surface area enables the active phase to be in contact with more of the reactants in the stream passing through the catalyst, and hence more of the reactants will take place in the catalytic reactions. The platinum catalyst with 4 g active phase per litre of monolith has a larger surface area than the platinum catalyst with 8 g active phase per litre of monolith. In terms of these catalyst activities both showed approximately the same activity for diesel fuel and unleaded petrol combustion. Both perovskite catalysts have similar surface areas and these catalysts both showed similar catalytic activity for the combustion of diesel fuel.

7.5 Reynolds numbers through the channels

As shown in the results (Chapters 5 & 6), the Reynolds numbers through the channels are in the transitional regime. The Reynolds number of the air and fuel mixture in the ¾ inch reactor tubing just prior to entering the catalysts is turbulent (approx 18,300). It can therefore be surmised that due to the short residence time (approximately 2.5×10^{-3} seconds) of the reactants travelling through the catalyst and because of entrance effects due to the reactants entering the narrow channels, the flow regime through the catalysts will remain turbulent.

7.6 Future Work.

In this thesis the catalytic combustion of unleaded petrol and diesel fuel were performed using platinum and perovskite catalysts. The perovskite catalysts showed little catalytic activity for the combustion of unleaded petrol over the range of inlet temperatures studied, and as shown in *Graph 7.1* the activity of the perovskite increased with increasing inlet temperature. Future work should be performed at higher inlet temperatures to establish if the perovskite catalyst shows greater catalytic activity at higher catalyst inlet temperatures.

When using methane as a fuel in the test rig all the catalysts studied showed little or no activity over the range of inlet temperatures studied, if the catalyst inlet temperature can be increased, in a future investigation, then activity for methane combustion may be noted. This would allow comparisons to be made with other studies that have been reported in the open literature.

The experiments described in this work were performed at Reynolds numbers equivalent to transitional flow through the catalysts. Future work is necessary to increase the Reynolds number through the catalyst channels to obtain true turbulent flow regimes. This can be achieved by reducing even further the diameter of the catalytic reaction section, or by increasing the air and fuel flowrates respectively.

The perovskite catalyst used in this research was $LaMnO_3$, which has been shown to have high catalytic activity for methane combustion. In future work the lanthanum and manganese ions could be changed and or substituted for other similar ions to investigate whether these ions have any influence on the catalytic combustion of unleaded petrol or diesel fuel.

It has been shown that unleaded petrol and diesel fuel are complex blends of many hydrocarbons, to obtain rate equations it would be necessary to try and simplify these fuels to a number of pure hydrocarbons, future work could look at simplifying the fuels to obtain approximate rate equations which could then be used to predict the activity for unleaded petrol and diesel fuel. This prediction could then be tested experimentally with unleaded petrol and diesel fuel to establish the validity of any such simplifications.

Finally the work detailed in this thesis should be scaled up and utilised as part of a full gas turbine system, to establish the commercial feasibility of such a system.

7.7 Overall conclusions

The overall key conclusions from the experimental work are summarised below:

7.7.1 Catalytic combustion of unleaded petrol

1. The perovskite catalyst with the greatest active phase loading (24 g $LaMnO_3$) showed no activity for the catalytic combustion of unleaded petrol
2. The rate of reaction is independent of catalyst inlet temperature for both of the platinum catalysts, and the industrial Degussa catalyst over the range of inlet temperatures studied.
3. The observed rate of reaction is dependent on the reactor pressure for both of the platinum catalysts and the industrial Degussa catalyst. Higher pressures show an increase in the observed rate of reaction, which is also shown by an increase in the temperature rise across the catalysts.
4. The Reynolds numbers through the catalyst channels remains unchanged with pressure, and are similar for both of the platinum and the industrial Degussa catalyst. The flow through the channels in the transitional regime.
5. The observed rate of reaction is dependent on the unleaded petrol flowrate for both of the platinum and the industrial Degussa catalyst. At low flowrates less of the available unleaded petrol is combusted than at high flowrates.
6. The observed rate of reaction increases with an increase in the total mass flowrate for both of the platinum catalysts. This indicates that the catalytic combustion is mass transfer limited even at the high Reynolds numbers seen through the catalyst channels.

7.7.2 Catalytic combustion of diesel fuel

1. The rate of reaction is independent of catalyst inlet temperature for both of the platinum catalysts, and the industrial Degussa catalyst over the range of inlet temperatures studied. The perovskite catalysts showed a dependency with catalyst inlet temperature, both perovskite catalysts showing no activity at temperatures below 380°C.
2. The observed rate of reaction is dependent on the reactor pressure for all of the catalysts studied. Higher pressures show an increase in the observed rate of reaction, which is also shown by an increase in the temperature rise across the catalysts.
3. The Reynolds numbers through the catalyst channels remains unchanged with pressure, and are similar for all the catalysts studied. The flow through the channels in the transitional regime.
4. The observed rate of reaction is dependent on the diesel fuel flowrate for all of the catalysts studied. At low flowrates less of the diesel fuel is combusted than at high flowrates.
5. The observed rate of reaction increases with an increase in the total mass flowrate for both of the perovskite catalysts and both of the platinum catalysts studied. This indicates that the catalytic combustion is mass transfer limited even at the high Reynolds numbers seen through the catalyst channels.

7.7.3 Catalytic combustion of methane

None of the catalysts studied showed any catalytic activity for the combustion of methane over the range of inlet temperatures studied.

7.7.4 Catalyst comparisons

1. The industrial Degussa catalyst showed the highest catalytic activity for the combustion of diesel fuel over the entire range of inlet temperatures studied. The platinum catalysts showed higher activity than the perovskite catalysts, apart from at very high inlet temperatures where the perovskite catalysts show comparable activity to the platinum catalysts.
2. The industrial Degussa catalyst showed the highest catalytic activity for the combustion of unleaded petrol over the entire range of inlet temperatures studied. The perovskite catalysts showed no catalytic activity for unleaded petrol
3. Both of the platinum catalysts and the industrial Degussa catalyst exhibited higher catalytic activity for the combustion of unleaded petrol then for diesel fuel.

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APPENDIX A

Environmental situation.

Large quantities of fossil fuels, oil, gas and coal are burnt to fill the urgent global requirement for energy conversion processes. The burning of such fuels causes vast amounts of pollution to be emitted to the environment on a daily basis. The main pollutant species are nitrogen oxides, unburned hydrocarbons, and particulates.

Oxides of Nitrogen (NO_x).

Nitrogen Oxides (NO_x), are a key reagent involved in the production of tropospheric ozone which is a prominent constituent of "photochemical smogs". The overall smog reaction mechanism is shown below :

$$NMHC + NO + h\nu \rightarrow NO_2 + \text{other products} \qquad \text{(Equation A.1)}$$

Where : NMHC denotes various reactive non-methane hydrocarbons (ethylene, butane, etc.),

$h\nu$ indicates a quantum of solar radiation of wavelength less than about 410 nm.

Ozone formation by this mechanism is possible because solar radiation dissociates the NO_2 formed in Equation A.1:

$$NO_2 + h\nu(\lambda \leq 410 \text{ nm}) \rightarrow NO + O \qquad \text{(Equation A.2)}$$

and the recombination of O with molecular oxygen then produces ozone :

$$O + O_2 \rightarrow O_3 \qquad \text{(Equation A.3)}$$

The rate of formation of ozone and other toxic products of smog chemistry can be controlled by changing the atmospheric concentrations of NO and NO_2 (i.e. NO_x emissions).

NO_x emissions are not only a key reagent in the production of photochemical smog, but when they come into contact with moisture they can combine to produce nitric acid, which has the effect of lowering the pH value of rain water causing acid rain.

Global NO_x sources are estimated to contribute a total of 35 - 58 × 10^{12} g of nitrogen per year [Bosch and Janssen 1988]. The main sources of NO_x in the lower atmosphere are shown in the following table.

Source	*10^{12} g N_2 /year*	*% of total*
Combustion of fossil fuels	10 - 22	28.5 – 44
Biomass Burning	20	57 40
Lightning	3 - 4	8.5 – 8
Stratosphere	1.6	4.5 – 3
Ammonia oxidation	0.6 - 2.5	1.5 – 3
Soil	0 - 8	

As shown the combustion of fossil fuels, are thus the most important sources of oxides of nitrogen. In the industrialised countries combustion of fossil fuels in cars and lorries has been shown to be responsible for the major part of this source of pollution (for a selection of industrialised countries mobile sources contribute to 45 - 60 % of the total NOx emissions) [Goldstein 1974, Duprey 1968].

The existence of seven oxides of nitrogen is known, NO, NO_2, NO_3, N_2O, N_2O_3, N_2O_4 and N_2O_5[Duprey 1968]. However, the combustion gas resulting from fossil fuel consists mainly of the oxides NO and NO_2, with NO representing 90 - 95 % of the total NO_x. Three types of NO_x can be distinguished in flue-gas:

- Thermal NO_x - Formed by fixation of atmospheric nitrogen;
- Fuel NO_x - Formed by the oxidation of nitrogen-containing compounds in the fuel;

Prompt NO_x - Formed by the oxidation of intermediate HCN.

Thermal NOx.

This type of NO_x formation is fully explained by the mechanism proposed by Zeldovich [1946].

$$O_2 + N_2 \leftrightarrow NO + N \qquad \text{(Equation A.4)}$$

$$N + O_2 \leftrightarrow NO + O \qquad \text{(Equation A.5)}$$

The effect of temperature on the rates of these reactions has been investigated by Sarofin and Flogan [1976]. At temperatures below 1800 K the rates of both reactions were found to be insignificant, where as above 1800 K, for every increase in flame temperature of approximately 40 K, the rate was found to double. It was also discovered that an increase in Oxygen or Nitrogen concentration enhances the rates of formation [Zeldovich 1946].

Fuel NO_x.

Fuel NO_x is formed from the gas phase oxidation of devolatilised Nitrogen present in the fuel, otherwise known as fuel bound Nitrogen. In this mechanism, the organic Nitrogen compounds form a complex which may then be attacked by OH radicals and NO molecules [Bosch and Janssen 1988]:

$$\text{N-complex} + OH \leftrightarrow NO + \text{other products} \qquad \text{(Equation A.6)}$$

$$\text{N-complex} + NO \leftrightarrow N_2 + \text{other products} \qquad \text{(Equation A.7)}$$

At normal flame combustion temperatures, it has been shown that the formation of fuel NO_x is independent of the temperature of the flame, and is insensitive to the form and nature in which the Nitrogen was bound to the fuel [e.g., Bosch and Janssen 1988, Prasad *et al.* 1984].

Prompt NO_x formation.

This mechanism arises from the reactions of fuel-derived radicals with N_2 which eventually lead to NO_x. An experimental study performed by Fenimore [1971] indicates that prompt NO_x formation was only detected in hydrocarbon flames. Hydrogen and Carbon monoxide flames produced no prompt NO_x. The following reactions involving hydrocarbon species was proposed:

$$CH + N_2 \leftrightarrow HCN + N \qquad \text{(Equation A.8)}$$

$$C + N_2 \leftrightarrow CN + N \qquad \text{(Equation A.9)}$$

As reviewed by Hayhurst and Vince [1980], the formation of prompt NO_x was known to be relatively independent of temperature and was more significant in fuel rich flames than in lean or stoichiometric flames at the same temperature.

Unburned Hydrocarbons.

Although some individual hydrocarbons might be of direct environmental significance in their own right, their main environmental effect lies in their joint role with NO_x as precursors for "photochemical smogs". The difficulty involved in assessing the relative importance of various types of hydrocarbon to smog chemistry is the fact that "hydrocarbons" is a generic term covering a wide range of chemical species. These vary widely in their potential for the generation of photochemical pollution and, while significant advances have been made in assigning a scale of photochemical reactivity to a large number of specific hydrocarbon species, knowledge of the chemical nature of individual hydrocarbon emissions is very limited. A further point arising from the diverse nature of hydrocarbon emissions is that the geographical location of sources takes on an added significance.

Particulate emissions.

Particulates are defined as small liquid and solid particles found in smoke, dust, fumes and mist. Suspended particles of 2-3 microns find their way into the lungs of people, potentially causing the symptoms of acute respiratory diseases. Particles in the troposphere can be generally characterised by their sources:

Natural continental sources.

This source of particlulates includes the following:

- Dust particles raised by the wind, having sizes above about 0.5 μm in diameter.
- Very small particles (D_p < 0.4 μm), resulting from photochemical reactions between ozone and hydrocarbons emitted from vegetation
- Very small particles (D_p < 0.4 μm) from photochemical reactions involving gases such as SO_2, H_2S, NH_3 and O_3
- Particles from volcanic eruptions.

Natural marine aerosol.

These particles result from the evaporation of sea spray, and have essentially the composition of sea salt (NaCl), and are in the size range $D_p > 0.5$ μm.

Man made aerosols.

This source consists of:

- Solid particles formed in combustion processes (smoke).
- Particles in the range D_p < 0.5 μm, which result from photochemical reactions involving unburned or partially burned hydrocarbons and oxides of nitrogen.

In terms of man made particulates, Environmental Protection Agency (EPA) figures for the United States show that particulate emissions are about 28×10^6 tons per year.

APPENDIX B

Authors	Fuels studied	Catalyst/support system	Operating Conditions	Purpose of Study
Pfefferle et *al.* 1975	Methane; Propane; Diesel fuel and synthetic gas mixture in air.	Catalyst : Englehard CATCOM - precious metal(s) - no further details. Catalyst support : Not disclosed Catalyst dimensions : Diameter = 0.025 m Length = 0.075-0.15m	$T_{g.in}$ = 483 - 873°K. P =1 - 10bar. U = 8 - 25 m/s. FAR = below 0.45.	To investigate the performance of a catalytically supported thermal combustion process and discuss the feasability of scale-up
Blazowski et *al.* 1975	JP-4 fuel.	Catalyst : Englehard industries - no further details. Catalyst support : Not disclosed. Catalyst dimensions : Diameter = 0.18m Length = 0.18m	$T_{g.in}$ = 555 - 650°K. P = 4 -11bar. U = 13.7-21.9 m/s. FAR = 0.015-0.024.	To demonstrate performance and capability of reducing emissions over a broad operating range.
Wapler et *al.* 1976	Propane in air	Catalyst : Pt. Catalyst support : Not disclosed. Catalyst dimensions : Diameter = 0.089 m Length=0.073,0.102m	$T_{g.in}$ = 700 - 730°K. P = atmospheric. FAR < 0.0185.	Evaluation of emission indexes and combustion efficiencies.

Siminski et *al.* 1976	JP-4 fuel	Catalyst : 35 different types. Catalyst support : Cordierete, SiC, metal foil, Ni alloy screens. Catalyst dimensions : Diameter = 0.0508 m Length = 0.216 m	$T_{g.in}$ > 400°K. P = 3.8 bar. U = 25.8 m/s.	To investigate the viability of operating inhybrid mode with a homogeneous combustion followed by a catalytic stage.
DeCorso et *al.* 1977	Distilate oil, syntheic coal gas in air	Catalyst : precious metal. Catalyst support : 3 monolith segments Catalyst dimensions : Diameter = 0.025 m Length=0.0508 m (X2) =0.0762 m (X1)	$T_{g.in}$ = 600 - 683°K. P = 3 -6 bar. U = 14.9 - 41.8 m/s. FAR = 0.026-0.028.	To study catalytically supported thermal combustion.
Enga and Thompson, 1979	Diesel, gasoline, kerosines, natural gas in air	Catalyst : Not disclosed. Catalyst support : Metallic monolith Catalyst dimensions : Diameter = 0.1016 m. Length=0.0762 m.	$T_{g.in}$ = 693°K. P = Not disclosed. U = 60 m/s. FAR = 0.34-0.4.	To test a catalytic combustor unit.

Osgerby et *al.* 1981	No 2 diesel fuel oil	Catalyst : Englehard CATCOM, Pd. Catalyst support : Not disclosed. Catalyst dimensions : two catalysts used each with 2 segments. Diameter of 1st = 0.0254 m. Length of 1st = 0.0762 m & 5m. Diameter of 2nd = 0.2286 m. Length of 2nd =0.0762 m & 0.0762 m.	$T_{g.in}$ = 633-723°K. P = atmospheric. U = 18 - 24 m/s.	To evaluate effects of catalyst length, inlet velocity and adiabatic temperature change on catalyst performance.
Anderson et *al* 1982	Gaseous and distillate fuels, No 2 diesel fuel in air	Catalyst : Chromium oxide and UOP, Inc. noble metal. Catalyst support : ceramic monolith Catalyst dimensions : Diameter = 0.13 m. 4 segments 0.0254 m long.	$T_{g.in}$ > 615°K. P = 1 - 5 bar. U = 6.1 - 15.3 m/s. FAR=0.0202-0.0278	To evaluate transient and steady state performance of a small-scale catalytic gas turbine combustor.
Prasad et *al* 1982	Propane and carbon monoxide in air.	Catalyst : Cr_2O_3 and CO_3O_4 on alumina. Catalyst support : ceramic monolith Catalyst dimensions : Ten 2 cm long monolith segments were used each separated by a 2 cm gap. Diameter = 0.10 m	$T_{g.in}$ = 633 - 661°K. P = Not disclosed. U = 4.4 - 7.3 m/s. FAR=0.02-0.16	To evaluate the kinetic parameters for the catalytic combustion of propane.

Bruno et *al* 1983	Propane in air.	Catalyst : Pt on γ alumina. Catalyst support : cordierite monolith Catalyst dimensions : Channel size = 0.024x0.024m^2. Length = 0.076 m.	$T_{g.in}$ = 650 - 800°K. P = 1.10 bar. U = 10 - 40 m/s. FAR=0.19 - 0.32	To study the relative importance of surface chemical and physical effects and of gas chemical kinetics for lean mixtures of propane and air.
Hoshino et *al* 1987	92 % Methane and 8 % Propane in air.	Catalyst : from the platinum metals group. Catalyst support : cordierite monolith Catalyst dimensions : Diameter = 0.18 m. Three segments of 2.5, 7.5 and 5 cm lengths.	$T_{g.in}$ > 623°K. U = 15 m/s.	To perform catalytic combustion engine tests to evaluate emission characteristics and to establish a system for control.
Furuya et *al* 1987	LNG (Liquified natural gas) and methane in air.	Catalyst : Pd and Pt on alumina. Catalyst support : cordierite monolith. Catalyst dimensions : Two different dimensions were used : a) diameter = 0.030 m length = 0.030 m (x5); b) diameter = 0.100 m, length = 0.030 m (x4).	$T_{g.in}$ = 573 - 873°K. P = 1 - 7 bar U = 10 - 35 m/s. FAR = 0.027.	To test the concept of a hybrid catalytic combustor.

Blumrich and Engler 1992	Methane and Oxygen in balanced Nitrogen.	Catalyst : Pd on alumina. Catalyst support : cordierite monolith. Catalyst dimensions : Not disclosed.	$T_{g.in}$ = 598 - 713°K P = Not disclosed $F_{air} = 5.55x10^{-4}$ m^3/s Fuel rich: 3% CH_4 & 5.88% O_2 Fuel lean: 3% CH_4 & 10.0% O_2	To investigate COP and NOx emissions from a laboratory-scale catalytic combustion system.
Quick and Kamitomati 1994	Natural gas in air.	Catalyst : 1st = PdO 2nd = PdO stabilised by rare earth oxides. Catalyst support : ceramic and fibre studied. Catalyst dimensions : Diameter = 0.0254 m 3 - 4 segmanets.	$T_{g.in}$ = 603 - 833°K P = 1 - 14 bar U = 3 -27 m/s FAR = 0.02 - 0.03	To test concept of hybrid design, turndown parameters, NOx emissions and catalyst life.
Griffin et *al* 1994	99.5% methane in air.	Catalyst : Pd based. Catalyst support : alumina based 250 cells/cm^2. Catalyst dimensions : Diameter = 0.075 m. Length = 0.075 m.	$T_{g.in}$ = 653°K P = atmospheric U = 10 m/s	To experimentally establish the use of catalytic combustion in NOx emissions reduction.

Hayashi et *al* 1994	Natural gas (98.5-98.9% methane).	Catalyst : Combinations of Pd, Pd/Pt and Pt. Catalyst support : cell densities varied from 15-31 cells/cm^2. Catalyst dimensions : Diameter = 0.100 m. 3 segments 2.5 cm in length.	$T_{g.in}$ = 773-973°K P = < 29 bar U = 12-20 m/s	To measure the effect of pressure on combustion efficiency and NOx formation.
Dalla Betta et *al* 1994	Natural gas (95.9% CH_4, 2.05% ethane).	Catalyst : Pd, on a high surface area mixed support. Catalyst support : corrugated FeCrAl metal foil monolith cell densities varied from 200-400 cells/in^2. Catalyst dimensions : Diameter = 0.055 m.	$T_{g.in}$ = 573-773°K P = < 14 bar	To demonstrate concept of a hybrid combustor, capable of operating at high pressures, with low emissions.
Furuya et *al* 1994	Natural gas.	Catalyst : a) Pd on alumina. b) Pd on alumina. Catalyst support : a) Cordierite b) Cordierite Catalyst dimensions : a) Dia = 0.45 m. b) Dia = 0.03 m	P : a) atmospheric b) 7 bar	To test catalyst performance at elevated pressure.

Sandamori et *al* 1994	Natural gas.	Catalyst : 7 segments. Segments 1,2 & 3 contain precious metals. Segments 4,5,6 and 7 contain Mn substituted hexaaluminate. Catalyst support : Segments 1,2 and 3 contain 31 cell/cm^2, the support being a cordierite honeycomb. Segments 4 and 5 contain 46 cell/cm^2, the support being a ceramic honeycomb sintered at 1200°C. Segments 6 and 7 contain 46 cell/cm^2, the support being a ceramic honeycomb sintered at 1300°C.`	$T_{g.in}$ = 723°K P = 10 bar U = < 9m/s	Performance of long term tests (215 hrs) to demonstrate the viability of a hybrid combustor.
Ozawa et *al* 1994	Natural gas (99.2% CH_4) LPG also studied.	Catalyst : Pd based on stabilised alumina. Catalyst support : Cordierite; cell pitch 3.3 mm Catalyst dimensions : Diameter = 0.22 m. Length = 0.025 m	$T_{g.in}$ = 723°K P = atmospheric.	To test catalyst combustor concep. In this design, premixed air and fuel are added to the homogeneous combustion section.

Vortmeyer et *al* 1996	Paraffins, alcohols and commercial fuels in air.	Not disclosed	$T_{g.in}$ = 544-767°K P = atmospheric.	To study a hybrid catalytic combustor.
Kolaczkowski et *al* 1996	Methane In air.	A proprietary catalyst-washcoat-monolith support system. Catalyst dimensions : Diameter = 0.117 m. Length = 0.051, 0.025, 0.0125 m	$T_{g.in}$ = 610 - 740°K P = atmospheric. F_{air}=0.28,0.73, 0.78 m^3/s $Y_{methane\ in}$ = 0.0094	To study heat and mass transfer for the catalytic combustion of methane under laminar flow and pseudo-steady state conditions.
Hayes et *al* 1996	Methane In air.	A proprietary catalyst-washcoat-monolith support system. Catalyst dimensions : Diameter = 0.117 m. Length = 0.025 - 0.151 m	$T_{g.in}$ = up to 881°K P = atmospheric. U = 1.7 m/s (at 288°K) $Y_{methane\ in}$=0.0046-0.0094	To study the catalytic combustion of methane in a monolith reactor under transient conditions.

Key to table : FAR = Fuel to air ratio P = Pressure $T_{gas\ in}$ = Temperature into combustor U = Velocity

$Y_{methane\ in}$ = Mole fraction of methane entering combustor.

APPENDIX C

Memorandum

BP Amoco

BP Amoco Oil
BP Oil International Limited
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Reference:

04 April 2000

Chris Flatley
Bath University
Dept of Chemical Engineering
BATH

BA2 7AY

Chris

Enclosed are the analyses for the ULG and DERV you sent me last week .

I Gasoline
Our analysis is carried out on a 100m 0.2mm column which explains the higher resolution. The major peaks are identified on the chromatogram (A & B). If you nee the smaller peaks let me know. The identifications up to and including TOLUENE are reliable. Above toluene there are too many isomers to identify the minor components. The major peaks at the back of the chromatogram are the C8-C10 aromatics.

II DERV
You will see that I get a lot more peaks than you do - this is probably due to the fact I use a direct injector and dilute the sample 1% in CS2. Using a splitter and a non diluted sample can and does cause problems with discrimination. I have quantified only the NORMAL ALKANES. This was done by integrating the peaks using a valley to valley mode and normalising each n-alkane to the total area of the sample. The column I used was a 30m, 0.2mm.

Both columns were non polar boiling point columns.

If you require any further information Email me on watt@bp.com.

Regards and good luck in the project

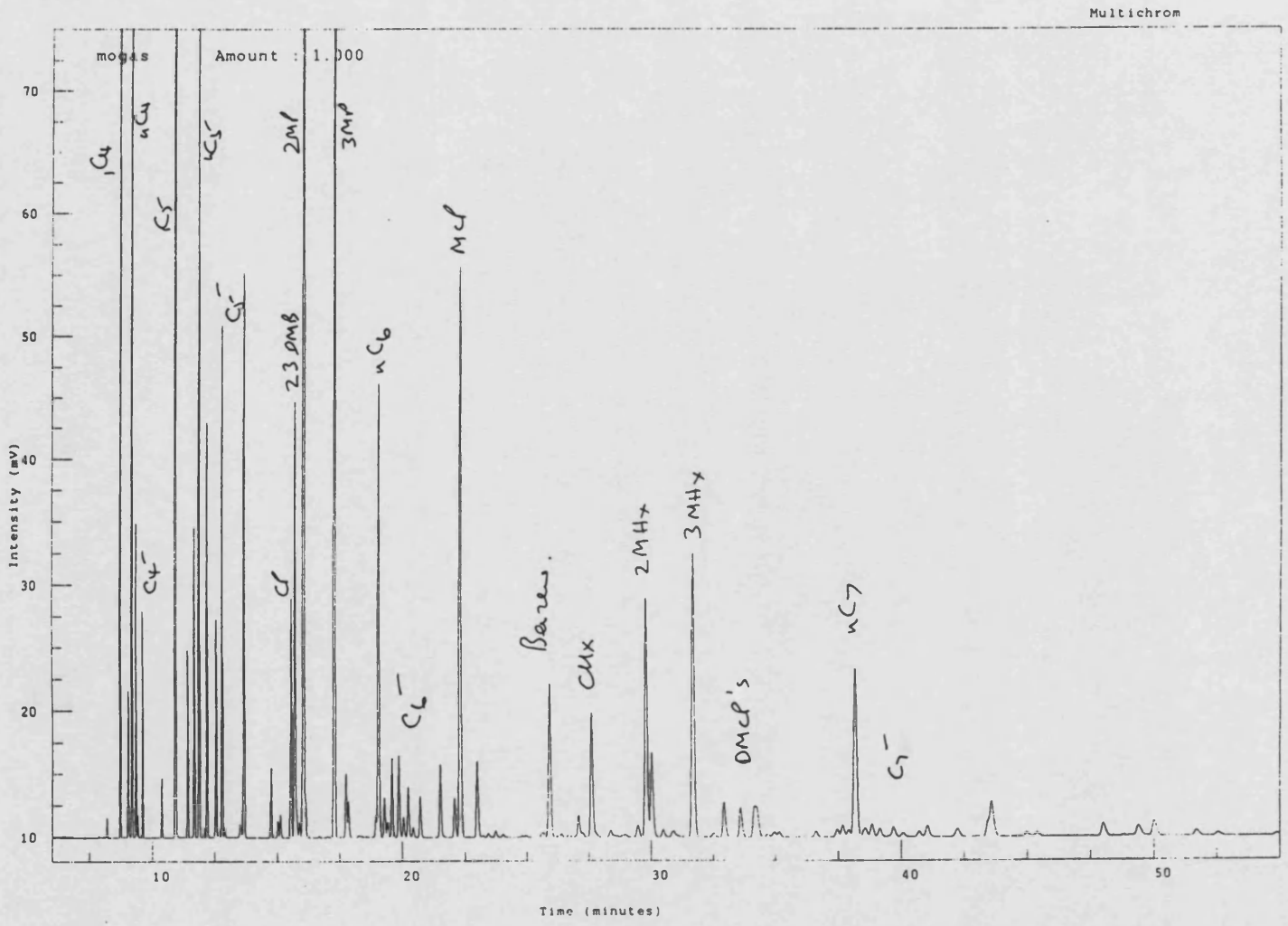
JERRY WATT

FUELS SAMPLE ANALYSIS: mogas

	% WT		% WT
Methane	0.00	2,4-Dimethylpentene-1	0.03
Ethane	0.00	1-Methylcyclopentene	0.00
Propane	0.03	Benzene	0.77
iso Butane	2.14	3-Methylhexene-1	0.01
iso butene + butene-1	0.27	3-Ethylpentene-1	0.01
Butadiene-1.3	0.00	3,3-Dimethylpentane	0.12
n Butane	3.03	2,4-Dimethylpentene-2	0.02
trans Butene-2	0.50	Cyclohexane	0.69
cis Butene-2	0.34	5-Methylhexene-1	0.00
Butadiene-1.2	0.00	2,3 Dimethylpentene-1	0.00
3-Methyl butene-1	0.10	trans 2-Methylhexene-3	0.05
iso Pentane	11.90	4-Methylhexene-1	0.02
Pentadiene-1.4	0.00	cis 4-Methylhexene-2	0.07
Pentene-1	0.35	2-Ethyl-3-methylbutene-1	
2-Methyl butene-1	0.60	trans 4-Methylhexene-2	
n Pentane	2.20	2-Methylhexane	1.40
isoprene	0.02	2,3 Dimethylpentane	0.52
trans Pentene-2	0.83	trans-5-Methylhexene-2	0.00
cis Pentene-2	0.48	1,1 Dimethylcyclopentane	0.04
2-Methyl butene-2	1.11	Cyclohexene	0.05
trans Pentadiene	0.02	3 Methylhexane	1.75
Cyclopentadiene	0.05	cis 3,4-Dimethylpentene-2	0.03
cis Pentadiene		1,cis 3-Dimethylcyclopentane	0.22
2,2 Dimethylbutane	1.39	1,trans 3-Dimethylcyclopentane	0.19
Cyclopentene	0.18	2-Methylhexene-1	0.00
4-Methyl pentene-1	0.04	1,trans 2-Dimethylcyclopentane	0.38
3-Methyl pentene-1	0.06	3-ethyl pentane	
Cyclopentane	0.66	trans 3,4-Dimethylcyclopentane	0.00
2,3 Dimethylbutane	1.28	2,2,4 Trimethylpentane	0.10
2,3 Dimethylbutene-1	0.04	Heptene-1	
cis 4-methylpentene-2	0.06	2-Ethylpentene-1	0.00
2 Methylpentane	4.75	trans 3-methylhexene-3	0.04
trans-4-methylpentene-2	0.11	trans Heptene-3	0.18
Hexadiene 1,5	0.00	n Heptane	1.25
3 Methylpentane	3.24	cis Heptene-3	0.08
2-methylpentene--1	0.20	trans 3-Methylhexene-2	0.00
Hexene-1	0.12	2-Methylhexene-2	0.09
?	0.06	cis 3-Methylhexene-3	0.06
n Hexane	1.57	trans Heptene-2	0.08
2 ethylbutene	0.05	3-Ethylpentene-2	0.03
cis/trans Hexene-3	0.13	?	0.04
trans Hexene-2	0.28	cis 3-Methylhexene-2	0.09
2 Methyl pentene-2	0.29	2,3-Dimethylpentene-2	0.08
3-Methylcyclopentene	0.07	cis Heptene-2	
4,4-Dimethylpentene-1	0.18	Methylcyclohexane	0.42
trans-3-Methylpentene-2		1,cis-2 Dimethylcyclopentane	
4-methylcyclopentene	0.04	2,2,3,3 Tetramethylbutane	
cis-Hexene-2	0.15	1,1,3 Trimethylcyclopentane	0.03
?	0.00	2,2-Dimethylhexane	0.03
cis-3-Methylpentene-2	0.29	Ethylcyclopentane	0.12
2,2 Dimethylpentane	0.16	3-Methylcyclohexene	0.00
Methylcyclopentane	2.40	4-Methylcyclohexene	0.00
trans-4,4-Dimethylpentene-2		2,5 Dimethylhexane	0.12
3,3-Dimethylpentene-1	0.35	2,2,3 Trimethylpentane	0.00
2,3-Dimethylbutene-2		2,4 Dimethylhexane	0.15
2,4 Dimethylpentane		1,trans,2 cis 4-Trimethylcyclopentane	0.06
Methylcyclopentadiene-2	0.02	3,3 Dimethylhexane	0.03
2,2,3 Trimethylbutene-1	0.00	1,trans,2,cis 3-Trimethylcyclopentane	0.02
Methylcyclopentadiene-1	0.00	2,3,4 Trimethylpentane	0.00
2,2,3 Trimethylbutane	0.03	Toluene	16.70
Methylcycopentadiene-3	0.01	2,3,3 Trimethylpentane	0.00
?	0.00	Ethanol	0.00
3,4-Dimethylpentene-1	0.00	MTBE	0.00
cis-4,4-Dimethylpentene-2	0.00	Higher Boilers	31.59
		TOTAL	100.00

Reported by: Date: Method of Test GCH/03

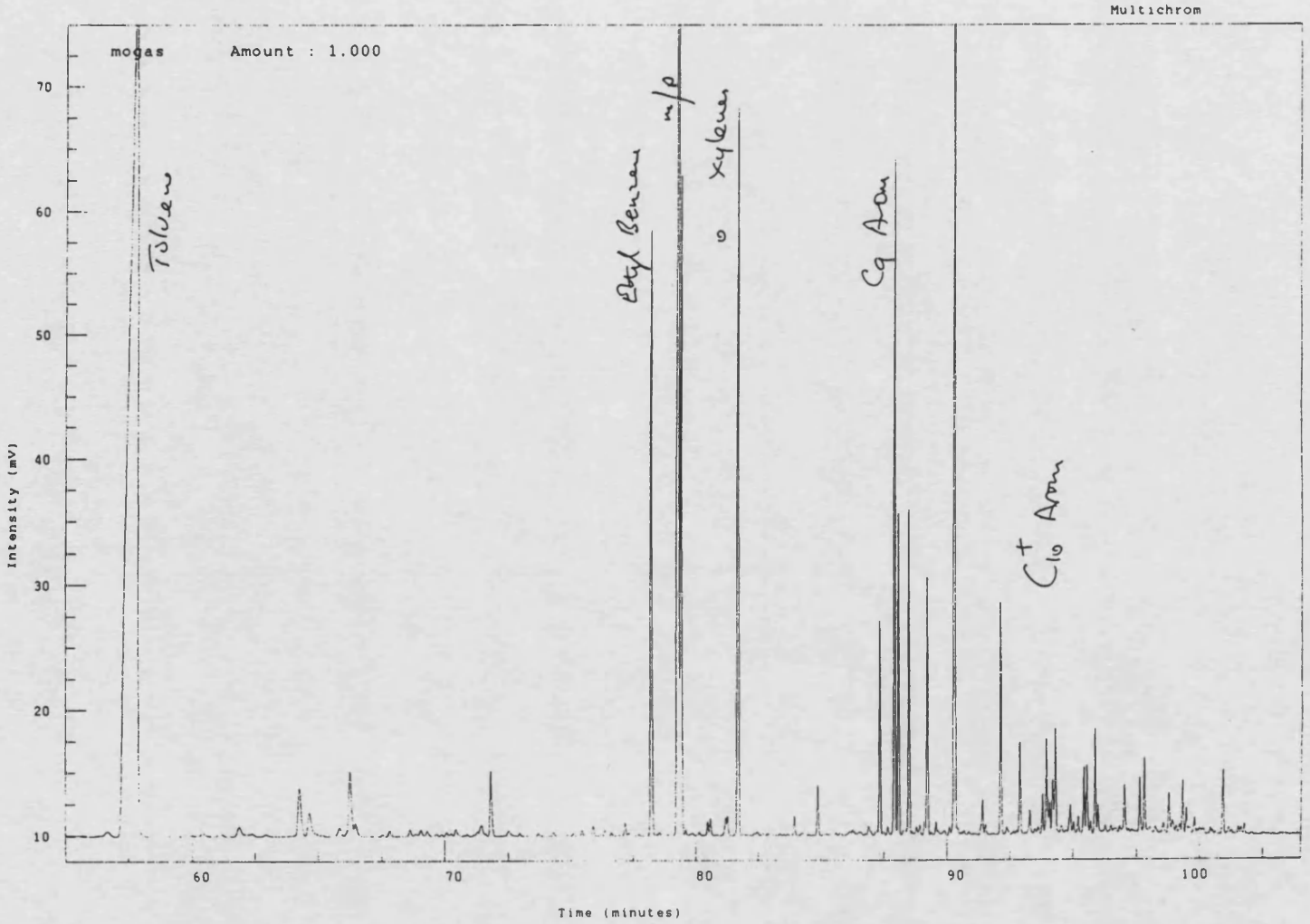
Analysis Name : [737] 69 SMC030400A,3,1.



Acquired on 3-APR-2000 at 16:18

Reported on 4-APR-2000 at 09:51

Analysis Name : [737] 69 SMC030400A,3,1.



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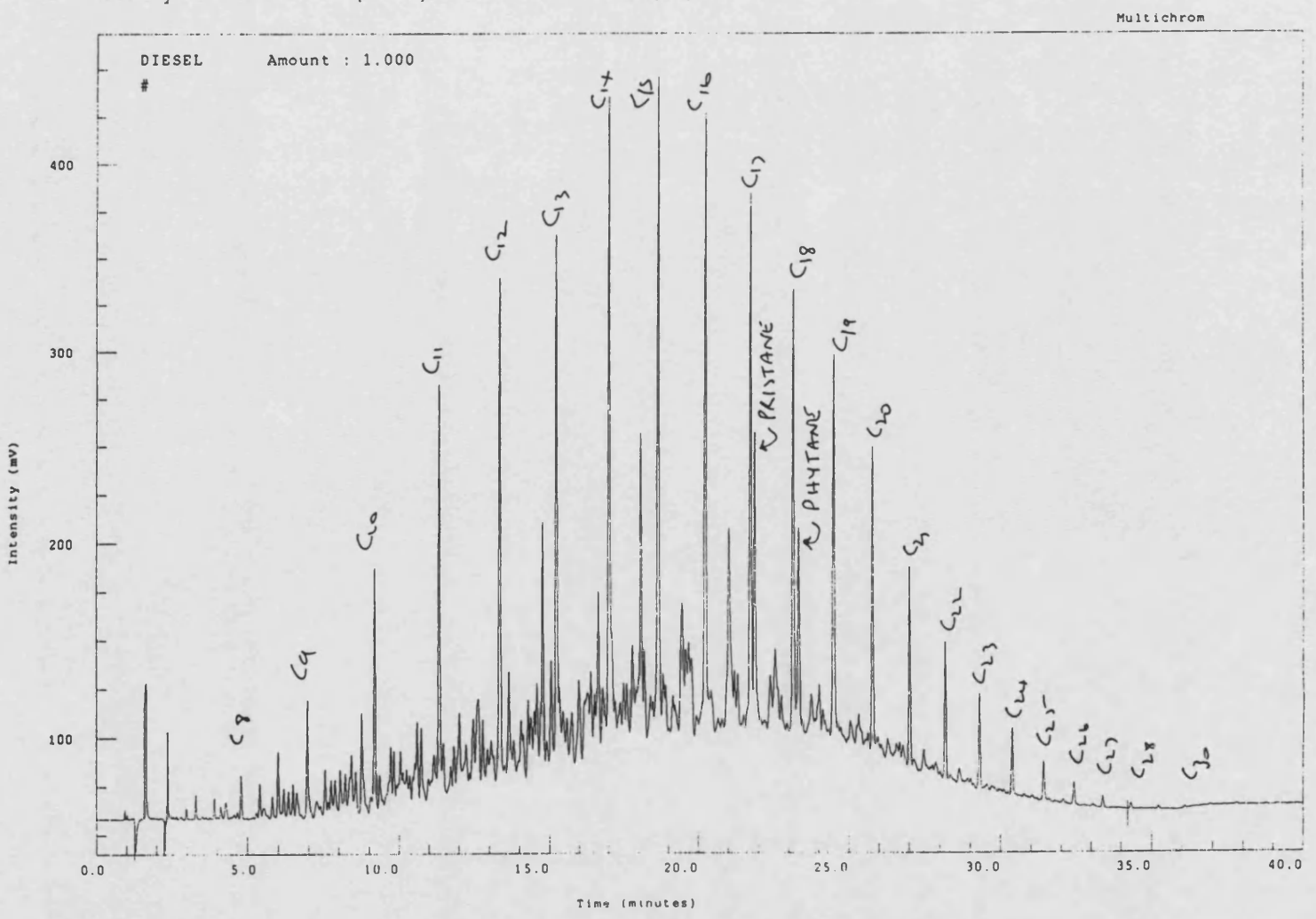

Acquired on 4-APR-2000 at 12:23 Reported on 4-APR-2000 at 15:48

NORMAL ALKANES	% wt/wt
7	0.10
8	0.36
9	0.66
10	1.03
11	1.52
12	1.58
13	2.11
14	2.06
15	1.89
16	1.55
17	1.28
18	1.19
19	0.83
20	0.55
21	0.38
22	0.27
23	0.20
24	0.07
25	0.04
26	0.02

APPENDIX D

Platinum 4g/l Petrol Effect of Inlet temperature - Run 1

Constants for calculations

Atmospheric pressure (bar)	1
Atmospheric temperature (°C)	20
Density of liquid Petrol (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Pt
Amount	4 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 12/09/2000 - Run 1

Reactor Pressure (barg)	2	2	2	2
Inlet set temperature (°C)	350	400	450	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	6.1	6.1	6.1	6.1
Actual inlet temp before Petrol added (°C)	334	381	428	476
Measured wall temp (°C)	334	381	428	475
Outlet temp before Petrol added (°C)	327	374	420	465
Actual inlet temp after Petrol added (°C)	331	387	428	473
Wall temp after Petrol added (°C)	435	468	504	588
Outlet temp after Petrol added (°C)	436	465	500	578
Inlet THC (ppm) (Volume basis)	4450	4350	4890	4200
Outlet (ppm) (Volume basis)	2680	2500	2610	2200

Calculated results for 12/09/2000 - Run 1

Conversion based on THC (Vol %)	39.7752809	42.52874	46.62577	47.61905
Temperature Change (°C)	105	78	72	105
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (kg/s)	7.45217E-05	7.45E-05	7.45E-05	7.45E-05
Total mass flow (Kg/s)	0.009995148	0.009995	0.009995	0.009995
Air to Fuel ratio (mol basis)	449.8675109	449.8675	449.8675	449.8675
Mols petrol in (mol/s)	0.000760425	0.00076	0.00076	0.00076
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	35	26	24	35
Mols combusted (mol/s)	0.000266149	0.000198	0.000183	0.000266
Obsevered reaction rate (mol/sm2)	**0.005061104**	**0.00376**	**0.00347**	**0.005061**
Density of air at reactor inlet (kg/m3)	1.732496212	1.585497	1.492764	1.402718
Velocity of air through a channel (m/s)	52.26714587	57.11311	60.66104	64.55512
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.08927E-05	3.28E-05	3.41E-05	3.55E-05
Reynolds Number through a channel - calculated at inlet conditions	2931.202967	2762.614	2654.836	2548.91

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.005751624**	**0.00615**	**0.006742**	**0.006886**

Platinum 4g/l Petrol Effect of Inlet temperature - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Petrol (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Pt
Amount	4 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 12/09/2000 - Run 2

Reactor Pressure (BarG)	2	2	2
Inlet set temperature (°C)	500	450	400
Air flowrate (l/min) (Evaluated at ATP)	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	6.1	6.1	6.1
Actual inlet temp before Petrol added (°C)	472	428	383
Measured wall temp (°C)	472	428	383
Outlet temp before Petrol added (°C)	469	425	383
Actual inlet temp after Petrol added (°C)	473	428	381
Wall temp after Petrol added (°C)	589	545	488
Outlet temp after Petrol added (°C)	582	537	484
Inlet THC (ppm) (Volume basis)	4080	3740	3830
Outlet (ppm) (Volume basis)	1940	1680	1910

Calculated results for 12/09/2000 - Run 2

Conversion based on THC (Vol %)	52.45098039	55.08021	50.13055
Temperature Change (°C)	109	109	103
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	7.45217E-05	7.45E-05	7.45E-05
Total mass flow (Kg/s)	0.009995148	0.009995	0.009995
Air to Fuel ratio (mol basis)	449.8675109	449.8675	449.8675
Mols petrol in (mol/s)	0.000760425	0.00076	0.00076
Adiabatic temp for 100% conversion (°C)	300	300	300
Conversion based on temp (%)	36.33333333	36.33333	34.33333
Mols combusted (mol/s)	0.000276288	0.000276	0.000261
Obsevered reaction rate (mol/sm2)	**0.005253908**	**0.005254**	**0.004965**
Density of air at reactor inlet (kg/m3)	1.402718113	1.492764	1.600042
Velocity of air through a channel (m/s)	64.55511725	60.66104	56.5939
Hydrolic mean diameter (m)	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.5526E-05	3.41E-05	3.26E-05
Reynolds Number through a channel - calculated at inlet conditions	2548.909989	2654.836	2779.413

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.007584568**	**0.007965**	**0.007249**

Platinum 8g/l Petrol Inlet temperature - Run 1

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid petrol fuel (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Pt
Amount	8 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 11/09/2000

Reactor Pressure (BarG)	2	2	2	2
Inlet set temperature (°C)	350	400	450	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	6.1	6.1	6.1	6.1
Actual inlet temp before petrol added (°C)	333	379	428	475
Measured wall temp (°C)	333	379	428	475
Outlet temp before petrol added (°C)	320	374	420	466
Actual inlet temp after petrol added (°C)	334	380	428	472
Wall temp after petrol added (°C)	483	489	555	622
Outlet temp after petrol added (°C)	468	506	543	618
Inlet THC (ppm) (Volume basis)	4900	3880	3100	3900
Outlet (ppm) (Volume basis)	2880	1930	1490	1800

Calculated results for 11/09/2000

Conversion based on THC (Vol %)	41.2244898	50.25773	51.93548	53.84615
Temperature Change (°C)	134	126	115	146
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	7.45217E-05	7.45E-05	7.45E-05	7.45E-05
Total mass flow (Kg/s)	0.009995148	0.009995	0.009995	0.009995
Air to Fuel ratio (mol basis)	449.8675109	449.8675	449.8675	449.8675
Mols petrol in (mol/s)	0.000760425	0.00076	0.00076	0.00076
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	44.66666667	42	38.33333	48.66667
Mols combusted (mol/s)	0.000339657	0.000319	0.000291	0.00037
Obsevered reaction rate (mol/sm2)	**0.006458933**	**0.006073**	**0.005543**	**0.007037**
Density of air at reactor inlet (kg/m3)	1.723933628	1.602493	1.492764	1.404601
Velocity of air through a channel (m/s)	52.5267509	56.50736	60.66104	64.46858
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.09958E-05	3.25E-05	3.41E-05	3.55E-05
Reynolds Number through a channel - calculated at inlet conditions	2921.449649	2782.24	2654.836	2551.139

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.005961184**	**0.007267**	**0.00751**	**0.007786**

Platinum 8g/l Petrol Inlet temperature - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid petrol fuel (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Pt
Amount	8 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 11/09/2000

Reactor Pressure (BarG)	2	2	2	2
Inlet set temperature (°C)	350	400	450	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6
Actual inlet temp before petrol added (°C)	333	382	430	474
Measured wall temp (°C)	333	382	430	474
Outlet temp before petrol added (°C)	324	374	422	472
Actual inlet temp after petrol added (°C)	332	381	429	474
Wall temp after petrol added (°C)	443	508	550	633
Outlet temp after petrol added (°C)	441	493	538	623
Inlet THC (ppm) (Volume basis)	3680	4060	4150	4410
Outlet (ppm) (Volume basis)	2000	2310	2200	2230

Calculated results for 11/09/2000

Conversion based on THC (Vol %)	45.65217391	43.10345	46.98795	49.43311
Temperature Change (°C)	109	112	109	149
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	6.84133E-05	6.84E-05	6.84E-05	6.84E-05
Total mass flow (Kg/s)	0.00998904	0.009989	0.009989	0.009989
Air to Fuel ratio (mol basis)	490.0342529	490.0343	490.0343	490.0343
Mols petrol in (mol/s)	0.000698095	0.000698	0.000698	0.000698
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	36.33333333	37.33333	36.33333	49.66667
Mols combusted (mol/s)	0.000253641	0.000261	0.000254	0.000347
Obsevered reaction rate (mol/sm2)	**0.00482326**	**0.004956**	**0.004823**	**0.006593**
Density of air at reactor inlet (kg/m3)	1.729632582	1.600042	1.490638	1.40084
Velocity of air through a channel (m/s)	52.35368088	56.5939	60.74758	64.64165
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.09271E-05	3.26E-05	3.41E-05	3.56E-05
Reynolds Number through a channel - calculated at inlet conditions	2927.941961	2779.413	2652.35	2546.686

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.006060338**	**0.005722**	**0.006238**	**0.006562**

Platinum 4g/l Petrol Pressure effects - Run 1

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Petrol (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Pt
Amount	4 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.05258711

Data for 12/09/2000 - Run 1

Reactor Pressure (BarG)	1.5	2	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	6.1	6.1	6.1	6.1	6.1
Actual inlet temp before Petrol added (°C)	476	476	476	476	474
Measured wall temp (°C)	476	475	475	476	474
Outlet temp before Petrol added (°C)	466	465	463	466	470
Actual inlet temp after Petrol added (°C)	471	473	472	472	474
Wall temp after Petrol added (°C)	568	588	601	609	643
Outlet temp after Petrol added (°C)	564	578	594	605	636
Inlet THC (ppm) (Volume basis)	4140	4200	4600	4540	4900
Outlet (ppm) (Volume basis)	2270	2200	2430	2160	2260

Calculated results for 12/09/2000

Conversion based on THC (Vol %)	45.1690821	47.619	47.1739	52.4229	53.8776
Temperature Change (°C)	93	105	122	133	162
Mass flowrate of Air (kg/s)	0.00992063	0.00992	0.00992	0.00992	0.00992
Mass flowrate of Fuel (Kg/s)	7.4522E-05	7.5E-05	7.5E-05	7.5E-05	7.5E-05
Air to Fuel ratio (mol basis)	449.867511	449.868	449.868	449.868	449.868
Mols petrol in (mol/s)	0.00076043	0.00076	0.00076	0.00076	0.00076
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	31	35	40.6667	44.3333	54
Mols combusted (mol/s)	0.00023573	0.00027	0.00031	0.00034	0.00041
Observered reaction rate (mol/sm2)	**0.004482692**	**0.005061**	**0.005881**	**0.006411**	**0.007809**
Density of air at reactor inlet (kg/m3)	1.17207405	1.40272	1.6387	1.8728	2.10126
Velocity of air through a channel (m/s)	77.2584567	64.5551	55.2588	48.3514	43.0944
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.5464E-05	3.6E-05	3.5E-05	3.5E-05	3.6E-05
Reynolds Number through a channel - calculated at inlet conditions	2553.37349	2548.91	2551.14	2551.14	2546.69

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.006531583**	**0.006886**	**0.006821**	**0.007581**	**0.007791**

Platinum 4g/l Petrol Pressure effects - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Petrol (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Pt
Amount	4 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.05258711

Data for 12/09/2000 - Run 2

Reactor Pressure (BarG)	1.5	2	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	6.1	6.1	6.1	6.1	6.1
Actual inlet temp before Petrol added (°C)	472	472	474	474	478
Measured wall temp (°C)	472	472	474	474	478
Outlet temp before Petrol added (°C)	468	469	470	470	473
Actual inlet temp after Petrol added (°C)	471	473	474	474	475
Wall temp after Petrol added (°C)	575	589	592	603	645
Outlet temp after Petrol added (°C)	570	582	583	600	635
Inlet THC (ppm) (Volume basis)	3870	4080	4060	4400	5150
Outlet (ppm) (Volume basis)	1855	1940	1870	1870	2330

Calculated results for 12/09/2000

Conversion based on THC (Vol %)	52.0671835	52.451	53.9409	57.5	54.7573
Temperature Change (°C)	99	109	109	126	160
Mass flowrate of Air (kg/s)	0.00992063	0.00992	0.00992	0.00992	0.00992
Mass flowrate of Fuel (Kg/s)	7.4522E-05	7.5E-05	7.5E-05	7.5E-05	7.5E-05
Air to Fuel ratio (mol basis)	449.867511	449.868	449.868	449.868	449.868
Mols petrol in (mol/s)	0.00076043	0.00076	0.00076	0.00076	0.00076
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	33	36.3333	36.3333	42	53.3333
Mols combusted (mol/s)	0.00025094	0.00028	0.00028	0.00032	0.00041
Obsevered reaction rate (mol/sm2)	**0.004771898**	**0.005254**	**0.005254**	**0.006073**	**0.007712**
Density of air at reactor inlet (kg/m3)	1.17207405	1.40272	1.63431	1.86779	2.09845
Velocity of air through a channel (m/s)	77.2584567	64.5551	55.4071	48.4812	43.1521
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.5464E-05	3.6E-05	3.6E-05	3.6E-05	3.6E-05
Reynolds Number through a channel - calculated at inlet conditions	2553.37349	2548.91	2546.69	2546.69	2544.47

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.007529069**	**0.007585**	**0.0078**	**0.008315**	**0.007918**

Platinum 8g/l Petrol Pressure effects - Run 1

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid petrol fuel (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Pt
Amount	8 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.05258711

Data for 11/09/2000

Reactor Pressure (BarG)	1.5	2	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	6.1	6.1	6.1	6.1	6.1
Actual inlet temp before petrol added (°C)	475	475	471	472	474
Measured wall temp (°C)	475	475	471	472	474
Outlet temp before petrol added (°C)	466	466	470	470	472
Actual inlet temp after petrol added (°C)	472	472	471	472	474
Wall temp after petrol added (°C)	595	622	664	672	711
Outlet temp after petrol added (°C)	613	618	642	655	683
Inlet THC (ppm) (Volume basis)	4550	3900	5500	5000	5000
Outlet (ppm) (Volume basis)	2100	1800	2450	1880	2030

Calculated results for 11/09/2000

Conversion based on THC (Vol %)	53.8461538	53.8462	55.4545	62.4	59.4
Temperature Change (°C)	141	146	171	183	209
Mass flowrate of Air (kg/s)	0.00992063	0.00992	0.00992	0.00992	0.00992
Mass flowrate of Fuel (Kg/s)	7.4522E-05	7.5E-05	7.5E-05	7.5E-05	7.5E-05
Air to Fuel ratio (mol basis)	449.867511	449.868	449.868	449.868	449.868
Mols petrol in (mol/s)	0.00076043	0.00076	0.00076	0.00076	0.00076
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	47	48.6667	57	61	69.6667
Mols combusted (mol/s)	0.0003574	0.00037	0.00043	0.00046	0.00053
Obsevered reaction rate (mol/sm2)	**0.00679634**	**0.007037**	**0.008242**	**0.008821**	**0.010074**
Density of air at reactor inlet (kg/m3)	1.1705008	1.4046	1.6409	1.8728	2.10126
Velocity of air through a channel (m/s)	77.3622987	64.4686	55.1846	48.3514	43.0944
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.5495E-05	3.5E-05	3.5E-05	3.5E-05	3.6E-05
Reynolds Number through a channel - calculated at inlet conditions	2551.13906	2551.14	2553.37	2551.14	2546.69

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.007786314**	**0.007786**	**0.008019**	**0.009023**	**0.008589**

Platinum 8g/l Petrol Pressure effects - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid petrol fuel (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Pt
Amount	8 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.05258711

Data for 11/09/2000

Reactor Pressure (BarG)	1.5	2	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6	5.6
Actual inlet temp before petrol added (°C)	472	474	472	474	480
Measured wall temp (°C)	472	474	472	474	480
Outlet temp before petrol added (°C)	470	472	471	472	472
Actual inlet temp after petrol added (°C)	472	474	472	474	477
Wall temp after petrol added (°C)	600	633	646	650	685
Outlet temp after petrol added (°C)	615	623	633	644	680
Inlet THC (ppm) (Volume basis)	4610	4410	5150	4900	5380
Outlet (ppm) (Volume basis)	2160	2230	2120	1800	2460

Calculated results for 11/09/2000

Conversion based on THC (Vol %)	53.1453362	49.4331	58.835	63.2653	54.2751
Temperature Change (°C)	143	149	161	170	203
Mass flowrate of Air (kg/s)	0.00992063	0.00992	0.00992	0.00992	0.00992
Mass flowrate of Fuel (Kg/s)	6.8413E-05	6.8E-05	6.8E-05	6.8E-05	6.8E-05
Air to Fuel ratio (mol basis)	490.034253	490.034	490.034	490.034	490.034
Mols petrol in (mol/s)	0.0006981	0.0007	0.0007	0.0007	0.0007
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	47.6666667	49.6667	53.6667	56.6667	67.6667
Mols combusted (mol/s)	0.00033276	0.00035	0.00037	0.0004	0.00047
Observered reaction rate (mol/sm2)	**0.006327763**	**0.006593**	**0.007124**	**0.007523**	**0.008983**
Density of air at reactor inlet (kg/m3)	1.1705008	1.40084	1.6387	1.86779	2.09286
Velocity of air through a channel (m/s)	77.3622987	64.6417	55.2588	48.4812	43.2675
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.5495E-05	3.6E-05	3.5E-05	3.6E-05	3.6E-05
Reynolds Number through a channel - calculated at inlet conditions	2551.13906	2546.69	2551.14	2546.69	2540.05

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.007055058**	**0.006562**	**0.00781**	**0.008398**	**0.007205**

Platinum 4g/l Petrol Fuel flowrate

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Petrol fuel (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Pt
Amount	4 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 12/09/2000

Reactor Pressure (BarG)	2	2	2
Inlet set temperature (°C)	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	3	6.1	4.6
Actual inlet temp before Petrol added (°C)	472	476	472
Measured wall temp (°C)	472	475	472
Outlet temp before Petrol added (°C)	470	465	470
Actual inlet temp after Petrol added (°C)	474	473	474
Wall temp after Petrol added (°C)	518	588	541
Outlet temp after Petrol added (°C)	517	578	536
Inlet THC (ppm) (Volume basis)	1550	4200	3160
Outlet (ppm) (Volume basis)	825	2200	1360

Calculated results for 12/09/2000

Conversion based on THC (Vol %)	46.77419355	47.61905	56.96203
Temperature Change (°C)	43	105	62
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921
Mass flowrate of Fuel (kg/s)	0.00003665	7.45E-05	5.62E-05
Total mass flow (kg/s)	0.009957277	0.009995	0.009977
Air to Fuel ratio (mol basis)	914.7306055	449.8675	596.5634
Mols diesel in (mol/s)	0.00037398	0.00076	0.000573
Adiabatic temp for 100% conversion (°C)	146.23	300	222.67
Conversion based on temp (%)	29.4057307	35	27.84389
Mols combusted (mol/s)	0.000109971	0.000266	0.00016
Obsevered reaction rate (mol/sm2)	**0.002091224**	**0.005061**	**0.003036**
Density of air at reactor inlet (kg/m3)	1.400840311	1.402718	1.40084
Velocity of air through a channel (m/s)	64.64165226	64.55512	64.64165
Hydrolic mean diameter (m)	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.5557E-05	3.55E-05	3.56E-05
Reynolds Number through a channel - calculated at inlet conditions	2546.686249	2548.91	2546.686

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.003326404**	**0.006886**	**0.006211**

Platinum 4g/l Petrol Total mass flow effects (Inlet temperature setpoint 500°C)

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Petrol fuel (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Pt
Amount	4 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 12/09/2000

Reactor Pressure (BarG)	2	2	3.5	3.5
Inlet set temperature (°C)	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	750	500	500	250
Fuel flowrate (ml/min) (Evaluated at ATP)	9	6	6	3
Actual inlet temp before Petrol added (°C)	475	476	474	467
Measured wall temp (°C)	475	475	474	467
Outlet temp before Petrol added (°C)	469	465	470	460
Actual inlet temp after Petrol added (°C)	468	473	474	471
Wall temp after Petrol added (°C)	667	588	643	613
Outlet temp after Petrol added (°C)	656	578	636	596
Inlet THC (ppm) (Volume basis)	6270	4200	4900	3900
Outlet (ppm) (Volume basis)	3090	2200	2260	1220

Calculated results for 12/09/2000

Conversion based on THC (Vol %)	50.71770335	47.61905	53.87755	68.71795
Temperature Change (°C)	188	105	162	125
Mass flowrate of Air (kg/s)	0.01488094	0.009921	0.009921	0.00496
Mass flowrate of Fuel (Kg/s)	0.00010995	7.33E-05	7.33E-05	3.67E-05
Total mass flow (Kg/s)	0.01499089	0.009994	0.009994	0.004997
Air to Fuel ratio (mol basis)	457.3653027	457.3653	457.3653	457.3653
Mols petrol in (mol/s)	0.001121939	0.000748	0.000748	0.000374
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	62.66666667	35	54	41.66667
Mols combusted (mol/s)	0.000703082	0.000262	0.000404	0.000156
Obsevered reaction rate (mol/sm2)	**0.013369848**	**0.004978**	**0.007681**	**0.002963**
Density of air at reactor inlet (kg/m3)	1.412183147	1.402718	2.10126	2.109733
Velocity of air through a channel (m/s)	96.1836633	64.55512	43.09443	21.46068
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.53706E-05	3.55E-05	3.56E-05	3.55E-05
Reynolds Number through a channel - calculated at inlet conditions	3840.163637	2548.91	2546.686	1276.687

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.010820553**	**0.006773**	**0.007663**	**0.004887**

Platinum 4g/l Petrol Total mass flow effects (inlet temperature setpoint 450°C)

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Petrol fuel (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Pt
Amount	4 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.05258711

Data for 12/09/2000

Reactor Pressure (BarG)	2	2	2	3.5	3.5
Inlet set temperature (°C)	450	450	450	450	450
Air flowrate (l/min) (Evaluated at ATP)	750	500	250	500	250
Fuel flowrate (ml/min) (Evaluated at ATP)	9	6	3	6	3
Actual inlet temp before Petrol added (°C)	433	428	426	428	426
Measured wall temp (°C)	433	428	426	428	426
Outlet temp before Petrol added (°C)	432	425	420	426	420
Actual inlet temp after Petrol added (°C)	420	428	428	429	427
Wall temp after Petrol added (°C)	634	545	565	599	626
Outlet temp after Petrol added (°C)	630	537	553	589	606
Inlet THC (ppm) (Volume basis)	6430	3740	3980	4380	4470
Outlet (ppm) (Volume basis)	2870	1680	1370	1920	1600

Calculated results for 12/09/2000

Conversion based on THC (Vol %)	55.3654743	55.0802	65.5779	56.1644	64.2058
Temperature Change (°C)	210	109	125	160	179
Mass flowrate of Air (kg/s)	0.01488094	0.00992	0.00496	0.00992	0.00496
Mass flowrate of Fuel (Kg/s)	0.00010995	7.3E-05	3.7E-05	7.3E-05	3.7E-05
Total mass flow (kg/s)	0.01499089	0.00999	0.005	0.00999	0.005
Air to Fuel ratio (mol basis)	457.365303	457.365	457.365	457.365	457.365
Mols petrol in (mol/s)	0.00112194	0.00075	0.00037	0.00075	0.00037
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	70	36.3333	41.6667	53.3333	59.6667
Mols combusted (mol/s)	0.00078536	0.00027	0.00016	0.0004	0.00022
Obsevered reaction rate (mol/sm2)	**0.014934405**	**0.005168**	**0.002963**	**0.007586**	**0.004243**
Density of air at reactor inlet (kg/m3)	1.5099967	1.49276	1.49276	2.23596	2.24235
Velocity of air through a channel (m/s)	89.9531426	60.661	30.3305	40.4984	20.1915
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.3852E-05	3.4E-05	3.4E-05	3.4E-05	3.4E-05
Reynolds Number through a channel - calculated at inlet conditions	4012.43812	2654.84	1327.42	2652.35	1328.66

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.011812149**	**0.007834**	**0.004664**	**0.007988**	**0.004566**

Platinum 4g/l Petrol Total mass flow effects (Inlet temperature setpoint 400°C)

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Petrol fuel (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Pt
Amount	4 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.05258711

Data for 12/09/2000

Reactor Pressure (BarG)	2	2	2	3.5	3.5
Inlet set temperature (°C)	400	400	400	400	400
Air flowrate (l/min) (Evaluated at ATP)	750	500	250	500	250
Fuel flowrate (ml/min) (Evaluated at ATP)	9	6	3	6	3
Actual inlet temp before Petrol added (°C)	383	383	382	382	388
Measured wall temp (°C)	383	383	382	382	388
Outlet temp before Petrol added (°C)	380	383	380	380	385
Actual inlet temp after Petrol added (°C)	377	381	382	382	383
Wall temp after Petrol added (°C)	549	488	526	530	556
Outlet temp after Petrol added (°C)	545	484	525	521	540
Inlet THC (ppm) (Volume basis)	6035	3830	3940	4690	4500
Outlet (ppm) (Volume basis)	3000	1910	1500	2030	1480

Calculated results for 12/09/2000

Conversion based on THC (Vol %)	50.2899751	50.1305	61.9289	56.7164	67.1111
Temperature Change (°C)	168	103	143	139	157
Mass flowrate of Air (kg/s)	0.01488094	0.00992	0.00496	0.00992	0.00496
Mass flowrate of Fuel (Kg/s)	0.00010995	7.3E-05	3.7E-05	7.3E-05	3.7E-05
Total mass flow (kg/s)	0.01499089	0.00999	0.005	0.00999	0.005
Air to Fuel ratio (mol basis)	457.365303	457.365	457.365	457.365	457.365
Mols petrol in (mol/s)	0.00112194	0.00075	0.00037	0.00075	0.00037
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	56	34.3333	47.6667	46.3333	52.3333
Mols combusted (mol/s)	0.00062829	0.00026	0.00018	0.00035	0.0002
Observered reaction rate (mol/sm2)	**0.011947524**	**0.004883**	**0.00339**	**0.00659**	**0.003722**
Density of air at reactor inlet (kg/m3)	1.60988879	1.60004	1.5976	2.3964	2.39275
Velocity of air through a channel (m/s)	84.3716345	56.5939	28.3402	37.787	18.9223
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.2447E-05	3.3E-05	3.3E-05	3.3E-05	3.3E-05
Reynolds Number through a channel - calculated at inlet conditions	4186.15246	2779.41	1388.3	2776.59	1386.89

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.010729298**	**0.00713**	**0.004404**	**0.008067**	**0.004773**

APPENDIX E

Perovskite 24g/l Petrol Inlet temperature - Run 1

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of Gasoline (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	LaMnO3
Amount	24 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 31/08/2000

Reactor Pressure (BarG)	2	2	2	2
Inlet set temperature (°C)	350	400	450	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	6.1	6.1	6.1	6.1
Actual inlet temp before Petrol added (°C)	336	380	430	476
Measured wall temp (°C)	336	380	430	476
Outlet temp before Petrol added (°C)	329	370	420	466
Actual inlet temp after Petrol added (°C)	336	380	430	476
Wall temp after Petrol added (°C)	336	380	430	476
Outlet temp after Petrol added (°C)	329	374	421	476
Inlet THC (ppm) (Volume basis)	4050	4100	4230	4700
Outlet (ppm) (Volume basis)	4040	4140	4240	4670

Calculated results for 31/08/2000

Conversion based on THC (Vol %)	0.24691358	-0.97561	-0.23641	0.638298
Temperature Change (°C)	-7	-6	-9	0
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	7.45217E-05	7.45E-05	7.45E-05	7.45E-05
Total mass flow (Kg/s)	0.009995148	0.009995	0.009995	0.009995
Air to Fuel ratio (mol basis)	449.8675109	449.8675	449.8675	449.8675
Mols petrol in (mol/s)	0.000760425	0.00076	0.00076	0.00076
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	-2.333333333	-2	-3	0
Mols combusted (mol/s)	-1.77433E-05	-1.5E-05	-2.3E-05	0
Obsevered reaction rate (mol/sm2)	**-0.000337407**	**-0.00029**	**-0.00043**	**0**
Density of air at reactor inlet (kg/m3)	1.718272106	1.602493	1.488517	1.3971
Velocity of air through a channel (m/s)	52.69982092	56.50736	60.83411	64.81472
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.10644E-05	3.25E-05	3.42E-05	3.56E-05
Reynolds Number through a channel - calculated at inlet conditions	2914.996608	2782.24	2649.87	2542.255

Based on analyser change

Observed rate of reaction (mol/sm2)	**3.57044E-05**	**-0.00014**	**-3.4E-05**	**9.23E-05**

Perovskite 24g/l Petrol Inlet temperature - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Petrol fuel (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	LaMnO3
Amount	24 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 31/08/2000

Reactor Pressure (BarG)	2	2	2
Inlet set temperature (°C)	450	400	350
Air flowrate (l/min) (Evaluated at ATP)	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	6.1	6.1	6.1
Actual inlet temp before Petrol added (°C)	432	384	340
Measured wall temp (°C)	432	384	340
Outlet temp before Petrol added (°C)	424	384	337
Actual inlet temp after Petrol added (°C)	432	384	338
Wall temp after Petrol added (°C)	432	384	338
Outlet temp after Petrol added (°C)	425	384	332
Inlet THC (ppm) (Volume basis)	4800	4270	4910
Outlet (ppm) (Volume basis)	4840	4300	4910

Calculated results for 31/08/2000

Conversion based on THC (Vol %)	-0.833333333	-0.70258	0
Temperature Change (°C)	-7	0	-6
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	7.45217E-05	7.45E-05	7.45E-05
Total mass flow (Kg/s)	0.009995148	0.009995	0.009995
Air to Fuel ratio (mol basis)	449.8675109	449.8675	449.8675
Mols petrol in (mol/s)	0.000760425	0.00076	0.00076
Adiabatic temp for 100% conversion (°C)	300	300	300
Conversion based on temp (%)	-2.333333333	0	-2
Mols combusted (mol/s)	-1.77433E-05	0	-1.5E-05
Obsevered reaction rate (mol/sm2)	**-0.000337407**	**0**	**-0.00029**
Density of air at reactor inlet (kg/m3)	1.484294627	1.592736	1.712648
Velocity of air through a channel (m/s)	61.00718185	56.8535	52.87289
Hydrolic mean diameter (m)	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.42363E-05	3.27E-05	3.11E-05
Reynolds Number through a channel - calculated at inlet conditions	2644.929135	2770.978	2908.582

Based on analyser change

Observed rate of reaction (mol/sm2)	**-0.000120502**	**-0.0001**	**0**

APPENDIX F

Degussa Petrol Inlet temperature - Run 1

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Unleaded petrol (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Degussa (Pt)
Amount	4 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 13/09/2000

Reactor Pressure (Barg)	2	2	2	2
Inlet set temperature (°C)	350	400	450	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	6.1	6.1	6.1	6.1
Actual inlet temp before Petrol added (°C)	334	382	429	474
Measured wall temp (°C)	334	382	429	474
Outlet temp before Petrol added (°C)	326	376	420	465
Actual inlet temp after Petrol added (°C)	333	380	427	473
Wall temp after Petrol added (°C)	512	553	597	636
Outlet temp after Petrol added (°C)	489	524	576	612
Inlet THC (ppm) (Volume basis)	4400	4320	4480	4360
Outlet (ppm) (Volume basis)	1720	1940	1720	1660

Calculated results for 13/09/2000

Conversion based on THC (Vol %)	60.90909091	55.09259	61.60714	61.92661
Temperature Change (°C)	156	144	149	139
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	7.45217E-05	7.45E-05	7.45E-05	7.45E-05
Total mass flow (Kg/s)	0.009995148	0.009995	0.009995	0.009995
Air to Fuel ratio (mol basis)	449.8675109	449.8675	449.8675	449.8675
Mols petrol in (mol/s)	0.000760425	0.00076	0.00076	0.00076
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	52	48	49.66667	46.33333
Mols combusted (mol/s)	0.000395421	0.000365	0.000378	0.000352
Obsevered reaction rate (mol/sm2)	**0.007519354**	**0.006941**	**0.007182**	**0.0067**
Density of air at reactor inlet (kg/m3)	1.726778403	1.602493	1.494897	1.402718
Velocity of air through a channel (m/s)	52.44021589	56.50736	60.57451	64.55512
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.09614E-05	3.25E-05	3.41E-05	3.55E-05
Reynolds Number through a channel - calculated at inlet conditions	2924.690872	2782.24	2657.329	2548.91

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.008807635**	**0.007967**	**0.008909**	**0.008955**

Degussa Petrol Inlet temperature - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Petrol fuel (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Degussa (Pt)
Amount	4 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 13/09/2000

Reactor Pressure (BarG)	2	2	2	2
Inlet set temperature (°C)	350	400	450	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	6.1	6.1	6.1	6.1
Actual inlet temp before Petrol added (°C)	333	385	431	475
Measured wall temp (°C)	333	385	431	475
Outlet temp before Petrol added (°C)	323	378	421	470
Actual inlet temp after Petrol added (°C)	333	382	428	472
Wall temp after Petrol added (°C)	484	537	578	625
Outlet temp after Petrol added (°C)	467	521	560	611
Inlet THC (ppm) (Volume basis)	4370	4080	4350	4270
Outlet (ppm) (Volume basis)	1840	1830	1735	1580

Calculated results for 13/09/2000

Conversion based on THC (Vol %)	57.89473684	55.14706	60.11494	62.99766
Temperature Change (°C)	134	139	132	139
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	7.45217E-05	7.45E-05	7.45E-05	7.45E-05
Total mass flow (Kg/s)	0.009995148	0.009995	0.009995	0.009995
Air to Fuel ratio (mol basis)	449.8675109	449.8675	449.8675	449.8675
Mols petrol in (mol/s)	0.000760425	0.00076	0.00076	0.00076
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	44.66666667	46.33333	44	46.33333
Mols combusted (mol/s)	0.000339657	0.000352	0.000335	0.000352
Obsevered reaction rate (mol/sm2)	**0.006458933**	**0.0067**	**0.006363**	**0.0067**
Density of air at reactor inlet (kg/m3)	1.726778403	1.5976	1.492764	1.404601
Velocity of air through a channel (m/s)	52.44021589	56.68043	60.66104	64.46858
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.09614E-05	3.26E-05	3.41E-05	3.55E-05
Reynolds Number through a channel - calculated at inlet conditions	2924.690872	2776.593	2654.836	2551.139

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.008371751**	**0.007974**	**0.008693**	**0.00911**

Degussa Petrol Pressure effects - Run 1

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Petrol fuel (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Degussa (Pt)
Amount	4 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.05258711

Data for 13/09/2000

Reactor Pressure (BarG)	1.5	2	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	6.1	6.1	6.1	6.1	6.1
Actual inlet temp before Petrol added (°C)	474	474	474	474	474
Measured wall temp (°C)	474	474	474	474	474
Outlet temp before Petrol added (°C)	465	465	469	469	470
Actual inlet temp after Petrol added (°C)	472	473	471	473	472
Wall temp after Petrol added (°C)	628	636	642	653	645
Outlet temp after Petrol added (°C)	609	612	625	636	641
Inlet THC (ppm) (Volume basis)	4420	4360	4230	4460	4760
Outlet (ppm) (Volume basis)	1690	1660	1600	1620	1690

Calculated results for 13/09/2000

Conversion based on THC (Vol %)	61.7647059	61.9266	62.1749	63.6771	64.4958
Temperature Change (°C)	137	139	154	163	169
Mass flowrate of Air (kg/s)	0.00992063	0.00992	0.00992	0.00992	0.00992
Mass flowrate of Fuel (Kg/s)	7.4522E-05	7.5E-05	7.5E-05	7.5E-05	7.5E-05
Air to Fuel ratio (mol basis)	449.867511	449.868	449.868	449.868	449.868
Mols petrol in (mol/s)	0.00076043	0.00076	0.00076	0.00076	0.00076
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	45.6666667	46.3333	51.3333	54.3333	56.3333
Mols combusted (mol/s)	0.00034726	0.00035	0.00039	0.00041	0.00043
Obsevered reaction rate (mol/sm2)	**0.006603536**	**0.0067**	**0.007423**	**0.007857**	**0.008146**
Density of air at reactor inlet (kg/m3)	1.1705008	1.40272	1.6409	1.87029	2.1069
Velocity of air through a channel (m/s)	77.3622987	64.5551	55.1846	48.4163	42.9791
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.5495E-05	3.6E-05	3.5E-05	3.6E-05	3.5E-05
Reynolds Number through a channel - calculated at inlet conditions	2551.13906	2548.91	2553.37	2548.91	2551.14

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.00893136**	**0.008955**	**0.008991**	**0.009208**	**0.009326**

Degussa Petrol Pressure effects - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Petrol fuel (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of petrol (g/mol)	98

Data on catalysts

Active phase	Degussa (Pt)
Amount	4 g/l
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.05258711

Data for 13/09/2000

Reactor Pressure (BarG)	1.5	2	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	6.1	6.1	6.1	6.1	6.1
Actual inlet temp before Petrol added (°C)	475	475	475	475	478
Measured wall temp (°C)	475	475	475	475	478
Outlet temp before Petrol added (°C)	470	470	474	473	476
Actual inlet temp after Petrol added (°C)	471	472	473	475	476
Wall temp after Petrol added (°C)	619	625	629	655	666
Outlet temp after Petrol added (°C)	608	611	618	633	643
Inlet THC (ppm) (Volume basis)	4330	4270	4480	4410	4550
Outlet (ppm) (Volume basis)	1710	1580	1730	1620	1570

Calculated results for 13/09/2000

Conversion based on THC (Vol %)	60.5080831	62.9977	61.3839	63.2653	65.4945
Temperature Change (°C)	137	139	145	158	167
Mass flowrate of Air (kg/s)	0.00992063	0.00992	0.00992	0.00992	0.00992
Mass flowrate of Fuel (kg/s)	7.4522E-05	7.5E-05	7.5E-05	7.5E-05	7.5E-05
Air to Fuel ratio (mol basis)	449.867511	449.868	449.868	449.868	449.868
Mols petrol in (mol/s)	0.00076043	0.00076	0.00076	0.00076	0.00076
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	45.6666667	46.3333	48.3333	52.6667	55.6667
Mols combusted (mol/s)	0.00034726	0.00035	0.00037	0.0004	0.00042
Obsevered reaction rate (mol/sm2)	**0.006603536**	**0.0067**	**0.006989**	**0.007616**	**0.00805**
Density of air at reactor inlet (kg/m3)	1.17207405	1.4046	1.6365	1.86529	2.09565
Velocity of air through a channel (m/s)	77.2584567	64.4686	55.333	48.5461	43.2098
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.5464E-05	3.5E-05	3.6E-05	3.6E-05	3.6E-05
Reynolds Number through a channel - calculated at inlet conditions	2553.37349	2551.14	2548.91	2544.47	2542.25

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.008749649**	**0.00911**	**0.008876**	**0.009148**	**0.009471**

APPENDIX G

Platinum 4g/l Diesel Inlet temperature - Run 1

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	3 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 07/09/2000

Reactor Pressure (BarG)	2	2	2	2
Inlet set temperature (°C)	350	400	450	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	330	380	430	476
Measured wall temp (°C)	330	380	430	476
Outlet temp before diesel added (°C)	320	374	425	471
Actual inlet temp after diesel added (°C)	330	379	456	487
Wall temp after diesel added (°C)	465	505	582	628
Outlet temp after diesel added (°C)	462	511	576	620
Inlet THC (ppm) (Volume basis)	1880	2850	2250	2600
Outlet (ppm) (Volume basis)	1000	1460	1241	1277

Calculated results for 07/09/2000

Conversion based on THC (Vol %)	46.80851064	48.77193	44.84444	50.88462
Temperature Change (°C)	132	132	120	133
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	0.0000784	7.84E-05	7.84E-05	7.84E-05
Total mass flow (Kg/s)	0.009999027	0.009999	0.009999	0.009999
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000392	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	44	44	40	44.33333
Mols combusted (mol/s)	0.00017248	0.000172	0.000157	0.000174
Obsevered reaction rate (mol/sm2)	**0.003279891**	**0.00328**	**0.002982**	**0.003305**
Density of air at reactor inlet (kg/m3)	1.73536934	1.60495	1.435429	1.376879
Velocity of air through a channel (m/s)	52.18061086	56.42083	63.08402	65.76661
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.08582E-05	3.25E-05	3.5E-05	3.6E-05
Reynolds Number through a channel - calculated at inlet conditions	2934.473936	2785.075	2587.547	2518.253

Based on analyser change

Observed reaction rate (mol/sm2)	**0.003489246**	**0.003636**	**0.003343**	**0.003793**

Platinum 4g/l Diesel Inlet temperature - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	3 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 07/09/2000

Reactor Pressure (BarG)	2	2
Inlet set temperature (°C)	450	400
Air flowrate (l/min) (Evaluated at ATP)	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6
Actual inlet temp before diesel added (°C)	429	380
Measured wall temp (°C)	429	380
Outlet temp before diesel added (°C)	428	372
Actual inlet temp after diesel added (°C)	455	379
Wall temp after diesel added (°C)	593	519
Outlet temp after diesel added (°C)	578	524
Inlet THC (ppm) (Volume basis)	2190	2105
Outlet (ppm) (Volume basis)	1245	1010

Calculated results for 07/09/2000

Conversion based on THC (Vol %)	43.15068493	52.019
Temperature Change (°C)	123	145
Mass flowrate of Air (kg/s)	0.009920627	0.009921
Mass flowrate of Fuel (Kg/s)	0.0000784	7.84E-05
Total mass flow (Kg/s)	0.009999027	0.009999
Air to Fuel ratio (mol basis)	872.6800471	872.68
Mols diesel in (mol/s)	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300
Conversion based on temp (%)	41	48.33333
Mols combusted (mol/s)	0.00016072	0.000189
Obsevered reaction rate (mol/sm2)	**0.003056263**	**0.003603**
Density of air at reactor inlet (kg/m3)	1.437400704	1.60495
Velocity of air through a channel (m/s)	62.99748708	56.42083
Hydrolic mean diameter (m)	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.49642E-05	3.25E-05
Reynolds Number through a channel - calculated at inlet conditions	2589.869922	2785.075

Based on analyser change

Observed reaction rate (mol/sm2)	**0.003216581**	**0.003878**

Platinum 8g/l Diesel inlet temperature - Run 1

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/molK)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	6 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 05/09/2000

Reactor Pressure (BarG)	2	2	2	2	2	2	2
Inlet set temperature (°C)	350	375	400	425	450	475	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	335	357	382	406	430	455	476
Measured wall temp (°C)	334	357	382	406	430	453	476
Outlet temp before diesel added (°C)	326	357	378	402	426	450	472
Actual inlet temp after diesel added (°C)	330	355	382	421	456	472	490
Wall temp after diesel added (°C)	518	533	556	604	628	654	669
Outlet temp after diesel added (°C)	502	523	548	590	606	626	651
Inlet THC (ppm) (Volume basis)	1500	1820	1615	1475	2160	2250	2480
Outlet (ppm) (Volume basis)	800	1100	951	890	1210	1210	965

Calculated results for 05/09/2000

Conversion based on THC (Vol %)	46.66666667	39.56044	41.11455	39.66102	43.98148	46.22222	61.08871
Temperature Change (°C)	172	168	164	169	150	154	161
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	0.0000784	7.84E-05	7.84E-05	7.84E-05	7.84E-05	7.84E-05	7.84E-05
Total mass flow (Kg/s)	0.009999027	0.009999	0.009999	0.009999	0.009999	0.009999	0.009999
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000392	0.000392	0.000392	0.000392	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300	300	300
Conversion based on temp (%)	57.33333333	56	54.66667	56.33333	50	51.33333	53.66667
Mols combusted (mol/s)	0.000224747	0.00022	0.000214	0.000221	0.000196	0.000201	0.00021
Observered reaction rate (mol/sm2)	**0.004273798**	**0.004174**	**0.004075**	**0.004199**	**0.003727**	**0.003827**	**0.004**
Density of air at reactor inlet (kg/m3)	1.73536934	1.666286	1.5976	1.507821	1.435429	1.404601	1.371465
Velocity of air through a channel (m/s)	52.18061086	54.34399	56.68043	60.0553	63.08402	64.46858	66.02621
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.08582E-05	3.17E-05	3.26E-05	3.39E-05	3.5E-05	3.55E-05	3.61E-05
Reynolds Number through a channel - calculated at inlet conditions	2934.473936	2855.58	2776.593	2672.421	2587.547	2551.139	2511.815

Based on analyser change

Observed reaction rate (mol/sm2)	**0.003478673**	**0.002949**	**0.003065**	**0.002956**	**0.003279**	**0.003446**	**0.004554**

Platinum 8g/l Diesel Inlet temperature - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	6 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 05/09/2000

Reactor Pressure (BarG)	2	2
Inlet set temperature (°C)	450	400
Air flowrate (l/min) (Evaluated at ATP)	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6
Actual inlet temp before diesel added (°C)	430	384
Measured wall temp (°C)	428	384
Outlet temp before diesel added (°C)	422	381
Actual inlet temp after diesel added (°C)	460	383
Wall temp after diesel added (°C)	595	510
Outlet temp after diesel added (°C)	578	527
Inlet THC (ppm) (Volume basis)	1840	1805
Outlet (ppm) (Volume basis)	845	830

Calculated results for 05/09/2000

Conversion based on THC (Vol %)	54.07608696	54.01662
Temperature Change (°C)	118	144
Mass flowrate of Air (kg/s)	0.009920627	0.009921
Mass flowrate of Fuel (Kg/s)	0.0000784	7.84E-05
Total mass flow (Kg/s)	0.009999027	0.009999
Air to Fuel ratio (mol basis)	872.6800471	872.68
Mols diesel in (mol/s)	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300
Conversion based on temp (%)	39.33333333	48
Mols combusted (mol/s)	0.000154187	0.000188
Obsevered reaction rate (mol/sm2)	**0.002932024**	**0.003578**
Density of air at reactor inlet (kg/m3)	1.427595788	1.595164
Velocity of air through a channel (m/s)	63.43016212	56.76697
Hydrolic mean diameter (m)	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.51209E-05	3.26E-05
Reynolds Number through a channel - calculated at inlet conditions	2578.311597	2773.782

Based on analyser change

Observed reaction rate (mol/sm2)	**0.004030993**	**0.004027**

Platinum 4g/l Diesel Pressure effects - Run 1

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	3 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.05258711

Data for 07/09/2000

Reactor Pressure (BarG)	1.5	2	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	476	476	478	478	478
Measured wall temp (°C)	476	476	477	477	478
Outlet temp before diesel added (°C)	472	471	476	476	475
Actual inlet temp after diesel added (°C)	484	487	490	496	497
Wall temp after diesel added (°C)	618	628	669	690	692
Outlet temp after diesel added (°C)	616	620	661	676	688
Inlet THC (ppm) (Volume basis)	2360	2600	2590	3100	3240
Outlet (ppm) (Volume basis)	1285	1277	1310	1200	1000

Calculated results for 07/09/2000

Conversion based on THC (Vol %)	45.5508475	50.8846	49.4208	61.2903	69.1358
Temperature Change (°C)	132	133	171	180	191
Mass flowrate of Air (kg/s)	0.00992063	0.00992	0.00992	0.00992	0.00992
Mass flowrate of Fuel (kg/s)	0.0000784	7.8E-05	7.8E-05	7.8E-05	7.8E-05
Air to Fuel ratio (mol basis)	872.680047	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.00039	0.00039	0.00039	0.00039
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	44	44.3333	57	60	63.6667
Mols combusted (mol/s)	0.00017248	0.00017	0.00022	0.00024	0.00025
Obsevered reaction rate (mol/sm2)	**0.003279891**	**0.003305**	**0.004249**	**0.004473**	**0.004746**
Density of air at reactor inlet (kg/m3)	1.15194596	1.37688	1.60004	1.81435	2.0385
Velocity of air through a channel (m/s)	78.6084028	65.7666	56.5939	49.9091	44.4213
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.5866E-05	3.6E-05	3.6E-05	3.6E-05	3.6E-05
Reynolds Number through a channel - calculated at inlet conditions	2524.73757	2518.25	2511.81	2499.07	2496.97

Based on analyser change

Observed reaction rate (mol/sm2)	**0.003395496**	**0.003793**	**0.003684**	**0.004569**	**0.005154**

Platinum 4g/l Pressure effects - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	3 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.05258711

Data for 07/09/2000

Reactor Pressure (BarG)	1.5	2	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	478	478	478	478	478
Measured wall temp (°C)	478	478	478	478	478
Outlet temp before diesel added (°C)	473	473	476	476	476
Actual inlet temp after diesel added (°C)	484	489	490	497	498
Wall temp after diesel added (°C)	625	633	672	692	698
Outlet temp after diesel added (°C)	619	625	667	678	687
Inlet THC (ppm) (Volume basis)	2155	2440	3000	2890	3600
Outlet (ppm) (Volume basis)	1080	1280	1560	1355	1365

Calculated results for 07/09/2000

Conversion based on THC (Vol %)	49.8839907	47.541	48	53.1142	62.0833
Temperature Change (°C)	135	136	177	181	189
Mass flowrate of Air (kg/s)	0.00992063	0.00992	0.00992	0.00992	0.00992
Mass flowrate of Fuel (Kg/s)	0.0000784	7.8E-05	7.8E-05	7.8E-05	7.8E-05
Air to Fuel ratio (mol basis)	872.680047	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.00039	0.00039	0.00039	0.00039
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	45	45.3333	59	60.3333	63
Mols combusted (mol/s)	0.0001764	0.00018	0.00023	0.00024	0.00025
Obsevered reaction rate (mol/sm2)	**0.003354434**	**0.003379**	**0.004398**	**0.004497**	**0.004696**
Density of air at reactor inlet (kg/m3)	1.15194596	1.37326	1.60004	1.812	2.03585
Velocity of air through a channel (m/s)	78.6084028	65.9397	56.5939	49.974	44.479
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.5866E-05	3.6E-05	3.6E-05	3.6E-05	3.6E-05
Reynolds Number through a channel - calculated at inlet conditions	2524.73757	2513.96	2511.81	2496.97	2494.86

Based on analyser change

Observed reaction rate (mol/sm2)	**0.003718502**	**0.003544**	**0.003578**	**0.003959**	**0.004628**

Platinum 8g/l Diesel Pressure effects - Run 1

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	6 wt %
Calcination temp (°C)	600
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.05258711

Data for 05/09/2000

Reactor Pressure (BarG)	1.5	2	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	478	476	477	481	480
Measured wall temp (°C)	476	476	477	481	479
Outlet temp before diesel added (°C)	472	472	476	481	478
Actual inlet temp after diesel added (°C)	486	490	490	495	502
Wall temp after diesel added (°C)	665	669	669	679	731
Outlet temp after diesel added (°C)	643	651	645	662	708
Inlet THC (ppm) (Volume basis)	2840	2480	2040	2335	2830
Outlet (ppm) (Volume basis)	1085	965	880	720	775

Calculated results for 05/09/2000

Conversion based on THC (Vol %)	61.7957746	61.0887	56.8627	69.1649	72.6148
Temperature Change (°C)	157	161	155	167	206
Mass flowrate of Air (kg/s)	0.00992063	0.00992	0.00992	0.00992	0.00992
Mass flowrate of Fuel (Kg/s)	0.0000784	7.8E-05	7.8E-05	7.8E-05	7.8E-05
Air to Fuel ratio (mol basis)	872.680047	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.00039	0.00039	0.00039	0.00039
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	52.3333333	53.6667	51.6667	55.6667	68.6667
Mols combusted (mol/s)	0.00020515	0.00021	0.0002	0.00022	0.00027
Obsevered reaction rate (mol/sm2)	**0.003901083**	**0.004**	**0.003851**	**0.00415**	**0.005119**
Density of air at reactor inlet (kg/m3)	1.14891053	1.37146	1.60004	1.81671	2.02534
Velocity of air through a channel (m/s)	78.8160869	66.0262	56.5939	49.8442	44.7098
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.5928E-05	3.6E-05	3.6E-05	3.6E-05	3.6E-05
Reynolds Number through a channel - calculated at inlet conditions	2520.40977	2511.81	2511.81	2501.18	2486.5

Based on analyser change

Observed reaction rate (mol/sm2)	**0.004606442**	**0.004554**	**0.004239**	**0.005156**	**0.005413**

Platinum 8g/l Diesel Pressure effects - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	6 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 05/09/2000

Reactor Pressure (BarG)	1.5	2	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	478	478	480	480	481
Measured wall temp (°C)	475	477	479	479	480
Outlet temp before diesel added (°C)	473	476	478	478	479
Actual inlet temp after diesel added (°C)	486	490	493	496	500
Wall temp after diesel added (°C)	638	657	665	696	739
Outlet temp after diesel added (°C)	625	642	648	674	707
Inlet THC (ppm) (Volume basis)	2660	2735	2580	3025	3060
Outlet (ppm) (Volume basis)	1385	1160	1110	980	995

Calculated results for 05/09/2000

Conversion based on THC (Vol %)	47.93233083	57.58684	56.97674	67.60331	67.48366
Temperature Change (°C)	139	152	155	178	207
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	0.0000784	7.84E-05	7.84E-05	7.84E-05	7.84E-05
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000392	0.000392	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	46.33333333	50.66667	51.66667	59.33333	69
Mols combusted (mol/s)	0.000181627	0.000199	0.000203	0.000233	0.00027
Obsevered reaction rate (mol/sm2)	**0.003453825**	**0.003777**	**0.003851**	**0.004423**	**0.005143**
Density of air at reactor inlet (kg/m3)	1.148910532	1.371465	1.593776	1.814352	2.030584
Velocity of air through a channel (m/s)	78.81608685	66.02621	56.81641	49.90907	44.59438
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.59277E-05	3.61E-05	3.61E-05	3.62E-05	3.64E-05
Reynolds Number through a channel - calculated at inlet conditions	2520.409769	2511.815	2505.421	2499.072	2490.674

Based on analyser change

Observed reaction rate (mol/sm2)	**0.003573019**	**0.004293**	**0.004247**	**0.005039**	**0.00503**

Platinum 4g/l Diesel Fuel flowrate

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	3 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 07/09/2000

Reactor Pressure (BarG)	2	2	2
Inlet set temperature (°C)	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	2.8	4.2	5.6
Actual inlet temp before diesel added (°C)	478	478	476
Measured wall temp (°C)	478	478	476
Outlet temp before diesel added (°C)	475	476	471
Actual inlet temp after diesel added (°C)	482	486	487
Wall temp after diesel added (°C)	571	617	628
Outlet temp after diesel added (°C)	566	603	620
Inlet THC (ppm) (Volume basis)	1680	1657	2600
Outlet (ppm) (Volume basis)	980	1020	1277

Calculated results for 07/09/2000

Conversion based on THC (Vol %)	41.66666667	38.44297	50.88462
Temperature Change (°C)	84	117	133
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921
Mass flowrate of Fuel (kg/s)	0.0000392	5.88E-05	7.84E-05
Total mass flow (kg/s)	0.009959827	0.009979	0.009999
Air to Fuel ratio (mol basis)	1745.360094	1163.573	872.68
Mols diesel in (mol/s)	0.000196	0.000294	0.000392
Adiabatic temp for 100% conversion (°C)	152	226	300
Conversion based on temp (%)	55.26315789	51.76991	44.33333
Mols combusted (mol/s)	0.000108316	0.000152	0.000174
Obsevered reaction rate (mol/sm2)	**0.00205974**	**0.002894**	**0.003305**
Density of air at reactor inlet (kg/m3)	1.38599697	1.378693	1.376879
Velocity of air through a channel (m/s)	65.33393234	65.68007	65.76661
Hydrolic mean diameter (m)	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.58045E-05	3.59E-05	3.6E-05
Reynolds Number through a channel - calculated at inlet conditions	2529.085798	2520.41	2518.253

Based on analyser change

Observed reaction rate (mol/s/m2)	**0.001552979**	**0.002149**	**0.003793**

Platinum 8g/l Diesel Fuel flowrate

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	6 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 05/09/2000

Reactor Pressure (BarG)	2	2	2
Inlet set temperature (°C)	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	2.8	4.2	5.6
Actual inlet temp before diesel added (°C)	478	478	476
Measured wall temp (°C)	477	478	476
Outlet temp before diesel added (°C)	473	473	472
Actual inlet temp after diesel added (°C)	484	478	490
Wall temp after diesel added (°C)	665	596	669
Outlet temp after diesel added (°C)	552	582	651
Inlet THC (ppm) (Volume basis)	1535	2230	2480
Outlet (ppm) (Volume basis)	700	1130	965

Calculated results for 05/09/2000

Conversion based on THC (Vol %)	54.39739414	49.32735	61.08871
Temperature Change (°C)	68	104	161
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	0.0000392	5.88E-05	7.84E-05
Total mass flow (Kg/s)	0.009959827	0.009979	0.009999
Air to Fuel ratio (mol basis)	1745.360094	1163.573	872.68
Mols diesel in (mol/s)	0.000196	0.000294	0.000392
Adiabatic temp for 100% conversion (°C)	152	226	300
Conversion based on temp (%)	44.73684211	46.0177	53.66667
Mols combusted (mol/s)	8.76842E-05	0.000135	0.00021
Obsevered reaction rate (mol/sm2)	**0.001667409**	**0.002573**	**0.004**
Density of air at reactor inlet (kg/m3)	1.382335155	1.393379	1.371465
Velocity of air through a channel (m/s)	65.50700236	64.98779	66.02621
Hydrolic mean diameter (m)	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.58662E-05	3.57E-05	3.61E-05
Reynolds Number through a channel - calculated at inlet conditions	2524.737567	2537.844	2511.815

Based on analyser change

Observed reaction rate (mol/sm2)	**0.002027472**	**0.002758**	**0.004554**

Platinum 4g/l Diesel Total mass flow effects 500°C

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	3 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.05258711

Data for 07/09/2000

Reactor Pressure (BarG)	2	2	2	3.5	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	750	500	250	500	250
Fuel flowrate (ml/min) (Evaluated at ATP)	8.4	5.6	2.8	5.6	2.8
Actual inlet temp before diesel added (°C)	477	476	471	478	472
Measured wall temp (°C)	477	476	471	478	472
Outlet temp before diesel added (°C)	472	471	465	475	465
Actual inlet temp after diesel added (°C)	489	487	481	497	489
Wall temp after diesel added (°C)	663	628	618	692	715
Outlet temp after diesel added (°C)	647	620	595	688	700
Inlet THC (ppm) (Volume basis)	2240	2600	1800	3240	3410
Outlet (ppm) (Volume basis)	1140	1277	825	1000	1240

Calculated results for 07/09/2000

Conversion based on THC (Vol %)	49.1071429	50.8846	54.1667	69.1358	63.6364
Temperature Change (°C)	158	133	114	191	211
Mass flowrate of Air (kg/s)	0.01488094	0.00992	0.00496	0.00992	0.00496
Mass flowrate of Fuel (Kg/s)	0.0001176	7.8E-05	3.9E-05	7.8E-05	3.9E-05
Total mass flow (Kg/s)	0.01499854	0.01	0.005	0.01	0.005
Air to Fuel ratio (mol basis)	872.680047	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000588	0.00039	0.0002	0.00039	0.0002
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	52.6666667	44.3333	38	63.6667	70.3333
Mols combusted (mol/s)	0.00030968	0.00017	7.4E-05	0.00025	0.00014
Obsevered reaction rate (mol/sm2)	**0.005888896**	**0.003305**	**0.001416**	**0.004746**	**0.002621**
Density of air at reactor inlet (kg/m3)	1.37326471	1.37688	1.38784	2.0385	2.0599
Velocity of air through a channel (m/s)	98.9095161	65.7666	32.6237	44.4213	21.9799
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.602E-05	3.6E-05	3.6E-05	3.6E-05	3.6E-05
Reynolds Number through a channel - calculated at inlet conditions	3770.93406	2518.25	1265.63	2496.97	1256.98

Based on analyser change

Observed reaction rate (mol/sm2)	**0.00549089**	**0.003793**	**0.002019**	**0.005154**	**0.002372**

Platinum 4g/l Diesel Total mass flow effects 450°C

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	3 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 07/09/2000

Reactor Pressure (BarG)	2	2	3.5	3.5
Inlet set temperature (°C)	450	450	450	450
Air flowrate (l/min) (Evaluated at ATP)	500	250	500	250
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	2.8	5.6	2.8
Actual inlet temp before diesel added (°C)	429	429	429	429
Measured wall temp (°C)	429	429	429	429
Outlet temp before diesel added (°C)	428	428	428	429
Actual inlet temp after diesel added (°C)	455	457	471	456
Wall temp after diesel added (°C)	593	585	674	647
Outlet temp after diesel added (°C)	578	583	654	613
Inlet THC (ppm) (Volume basis)	2190	2120	2980	2780
Outlet (ppm) (Volume basis)	1245	855	1245	1040

Calculated results for 07/09/2000

Conversion based on THC (Vol %)	43.15068493	59.66981	58.22148	62.58993
Temperature Change (°C)	123	126	183	157
Mass flowrate of Air (kg/s)	0.009920627	0.00496	0.009921	0.00496
Mass flowrate of Fuel (Kg/s)	0.0000784	3.92E-05	7.84E-05	3.92E-05
Total mass flow (kg/s)	0.009999027	0.005	0.009999	0.005
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000196	0.000392	0.000196
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	41	42	61	52.33333
Mols combusted (mol/s)	0.00016072	8.23E-05	0.000239	0.000103
Obsevered reaction rate (mol/sm2)	**0.003056263**	**0.001565**	**0.004547**	**0.001951**
Density of air at reactor inlet (kg/m3)	1.437400704	1.433463	2.109733	2.153143
Velocity of air through a channel (m/s)	62.99748708	31.58528	42.92136	21.02801
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.49642E-05	3.5E-05	3.55E-05	3.5E-05
Reynolds Number through a channel - calculated at inlet conditions	2589.869922	1292.615	2553.373	1293.773

Based on analyser change

Observed reaction rate (mol/sm2)	**0.003216581**	**0.002224**	**0.00434**	**0.002333**

Platinum 4g/l Diesel Total mass flow effects 400°C

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	3 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 07/09/2000

Reactor Pressure (BarG)	2	2	3.5	3.5
Inlet set temperature (°C)	400	400	400	400
Air flowrate (l/min) (Evaluated at ATP)	500	250	500	250
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	2.8	5.6	2.8
Actual inlet temp before diesel added (°C)	380	383	383	383
Measured wall temp (°C)	380	383	383	383
Outlet temp before diesel added (°C)	372	383	372	382
Actual inlet temp after diesel added (°C)	379	396	438	437
Wall temp after diesel added (°C)	519	542	650	607
Outlet temp after diesel added (°C)	524	548	623	592
Inlet THC (ppm) (Volume basis)	2105	1830	2325	1800
Outlet (ppm) (Volume basis)	1010	790	1050	805

Calculated results for 07/09/2000

Conversion based on THC (Vol %)	52.01900238	56.8306	54.83871	55.27778
Temperature Change (°C)	145	152	185	155
Mass flowrate of Air (kg/s)	0.009920627	0.00496	0.009921	0.00496
Mass flowrate of Fuel (kg/s)	0.0000784	3.92E-05	7.84E-05	3.92E-05
Total mass flow (kg/s)	0.009999027	0.005	0.009999	0.005
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000196	0.000392	0.000196
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	48.33333333	50.66667	61.66667	51.66667
Mols combusted (mol/s)	0.000189467	9.93E-05	0.000242	0.000101
Obsevered reaction rate (mol/sm2)	**0.003602911**	**0.001888**	**0.004597**	**0.001926**
Density of air at reactor inlet (kg/m3)	1.604950479	1.564167	2.207653	2.210763
Velocity of air through a channel (m/s)	56.42082634	28.94596	41.01759	20.47995
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.25135E-05	3.31E-05	3.44E-05	3.44E-05
Reynolds Number through a channel - calculated at inlet conditions	2785.074575	1368.965	2630.257	1316.344

Based on analyser change

Observed reaction rate (mol/sm2)	**0.003877652**	**0.002118**	**0.004088**	**0.00206**

Platinum 8g/l Diesel Total mass flow effects 500°C

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	6 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 05/09/2000

Reactor Pressure (BarG)	2	2	2	3.5	3.5	3.5
Inlet set temperature (°C)	500	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	750	500	250	750	500	250
Fuel flowrate (ml/min) (Evaluated at ATP)	8.4	5.6	2.8	8.4	5.6	2.8
Actual inlet temp before diesel added (°C)	477	476	478	478	480	468
Measured wall temp (°C)	476	476	478	478	479	465
Outlet temp before diesel added (°C)	471	472	478	476	478	451
Actual inlet temp after diesel added (°C)	491	490	486	501	502	485
Wall temp after diesel added (°C)	648	669	638	688	731	639
Outlet temp after diesel added (°C)	633	651	623	674	708	618
Inlet THC (ppm) (Volume basis)	2930	2480	1570	3560	2830	2750
Outlet (ppm) (Volume basis)	1360	965	775	1450	775	860

Calculated results for 05/09/2000

Conversion based on THC (Vol %)	53.58361775	61.08871	50.63694	59.26966	72.61484	68.72727
Temperature Change (°C)	142	161	137	173	208	133
Mass flowrate of Air (kg/s)	0.01488094	0.009921	0.00496	0.014881	0.009921	0.00496
Mass flowrate of Fuel (Kg/s)	0.0001176	7.84E-05	3.92E-05	0.000118	7.84E-05	3.92E-05
Total mass flow (Kg/s)	0.01499854	0.009999	0.005	0.014999	0.009999	0.005
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000588	0.000392	0.000196	0.000588	0.000392	0.000196
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300	300
Conversion based on temp (%)	47.33333333	53.66667	45.66667	57.66667	68.66667	44.33333
Mols combusted (mol/s)	0.00027832	0.00021	8.95E-05	0.000339	0.000269	8.69E-05
Obsevered reaction rate (mol/sm2)	**0.005292552**	**0.004**	**0.001702**	**0.006448**	**0.005119**	**0.001652**
Density of air at reactor inlet (kg/m3)	1.36966978	1.371465	1.378693	2.027961	2.025344	2.070767
Velocity of air through a channel (m/s)	99.16912114	66.02621	32.84004	66.9781	44.70976	21.86451
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.60814E-05	3.61E-05	3.59E-05	3.64E-05	3.64E-05	3.59E-05
Reynolds Number through a channel - calculated at inlet conditions	3764.517954	2511.815	1260.205	3732.88	2486.504	1261.286

Based on analyser change

Observed reaction rate (mol/sm2)	**0.005991424**	**0.004554**	**0.001887**	**0.006627**	**0.005413**	**0.002562**

Platinum 8g/l Diesel Total mass flow effects 450°C

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	6 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 05/09/2000

Reactor Pressure (BarG)	2	2	2	3.5	3.5	3.5
Inlet set temperature (°C)	450	450	450	450	450	450
Air flowrate (l/min) (Evaluated at ATP)	750	500	250	750	500	250
Fuel flowrate (ml/min) (Evaluated at ATP)	8.4	5.6	2.8	8.4	5.6	2.8
Actual inlet temp before diesel added (°C)	430	430	436	433	435	433
Measured wall temp (°C)	429	428	436	433	435	433
Outlet temp before diesel added (°C)	422	422	436	433	435	433
Actual inlet temp after diesel added (°C)	459	460	467	474	472	458
Wall temp after diesel added (°C)	611	595	618	675	656	614
Outlet temp after diesel added (°C)	600	578	601	646	627	594
Inlet THC (ppm) (Volume basis)	1910	1840	2050	2660	2730	2180
Outlet (ppm) (Volume basis)	970	845	800	1335	1130	960

Calculated results for 05/09/2000

Conversion based on THC (Vol %)	49.21485969	54.07609	60.97561	49.81203	58.60606	55.9633
Temperature Change (°C)	141	118	134	172	155	136
Mass flowrate of Air (kg/s)	0.01488094	0.009921	0.00496	0.014881	0.009921	0.00496
Mass flowrate of Fuel (Kg/s)	0.0001176	7.84E-05	3.92E-05	0.000118	7.84E-05	3.92E-05
Total mass flow (kg/s)	0.01499854	0.009999	0.005	0.014999	0.009999	0.005
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000588	0.000392	0.000196	0.000588	0.000392	0.000196
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300	300
Conversion based on temp (%)	47	39.33333	44.66667	57.33333	51.66667	45.33333
Mols combusted (mol/s)	0.00027636	0.000154	8.75E-05	0.000337	0.000203	8.89E-05
Obsevered reaction rate (mol/sm2)	**0.005255281**	**0.002932**	**0.001665**	**0.006411**	**0.003851**	**0.00169**
Density of air at reactor inlet (kg/m3)	1.429546055	1.427596	1.414092	2.10126	2.106901	2.147252
Velocity of air through a channel (m/s)	95.01544067	63.43016	32.01795	64.64165	42.97905	21.0857
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.50896E-05	3.51E-05	3.53E-05	3.56E-05	3.55E-05	3.51E-05
Reynolds Number through a channel - calculated at inlet conditions	3870.917914	2578.312	1281.183	3820.029	2551.139	1291.459

Based on analyser change

Observed reaction rate (mol/sm2)	**0.005502912**	**0.004031**	**0.002273**	**0.00557**	**0.004369**	**0.002086**

Platinum 8g/l Diesel Total mass flow effects 400°C

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	Pt
Amount	6 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 05/09/2000

Reactor Pressure (BarG)	2	2	3.5	3.5
Inlet set temperature (°C)	400	400	400	400
Air flowrate (l/min) (Evaluated at ATP)	500	250	500	250
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	2.8	5.6	2.8
Actual inlet temp before diesel added (°C)	384	384	386	386
Measured wall temp (°C)	384	383	386	386
Outlet temp before diesel added (°C)	381	377	386	386
Actual inlet temp after diesel added (°C)	383	411	445	440
Wall temp after diesel added (°C)	510	567	639	666
Outlet temp after diesel added (°C)	527	551	615	623
Inlet THC (ppm) (Volume basis)	1805	2150	1555	2300
Outlet (ppm) (Volume basis)	830	1080	640	850

Calculated results for 05/09/2000

Conversion based on THC (Vol %)	54.0166205	49.76744	58.84244	63.04348
Temperature Change (°C)	144	140	170	183
Mass flowrate of Air (kg/s)	0.009920627	0.00496	0.009921	0.00496
Mass flowrate of Fuel (Kg/s)	0.0000784	3.92E-05	7.84E-05	3.92E-05
Total mass flow (kg/s)	0.009999027	0.005	0.009999	0.005
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000196	0.000392	0.000196
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	48	46.66667	56.66667	61
Mols combusted (mol/s)	0.00018816	9.15E-05	0.000222	0.00012
Obsevered reaction rate (mol/sm2)	**0.003578063**	**0.001739**	**0.004224**	**0.002274**
Density of air at reactor inlet (kg/m3)	1.595164196	1.529865	2.18613	2.201461
Velocity of air through a channel (m/s)	56.76696638	29.59497	41.42142	20.56649
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.26459E-05	3.36E-05	3.46E-05	3.45E-05
Reynolds Number through a channel - calculated at inlet conditions	2773.782051	1349.052	2613.419	1312.708

Based on analyser change

Observed reaction rate (mol/sm2)	**0.00402656**	**0.001855**	**0.004386**	**0.00235**

APPENDIX H

Perovskite 8g/l Diesel Inlet temperature - Run 1

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	LaMnO3
Amount	8 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 06/09/2000

Reactor Pressure (BarG)	2	2	2	2	2	2	2
Inlet set temperature (°C)	350	375	400	425	450	475	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	332	359	379	406	430	451	478
Measured wall temp (°C)	332	359	379	406	430	451	478
Outlet temp before diesel added (°C)	322	350	371	399	424	451	468
Actual inlet temp after diesel added (°C)	333	359	381	428	459	473	489
Wall temp after diesel added (°C)	333	359	390	459	491	512	531
Outlet temp after diesel added (°C)	323	352	385	457	499	525	544
Inlet THC (ppm) (Volume basis)	2670	1910	1895	1860	2190	2510	2400
Outlet (ppm) (Volume basis)	2660	1910	1885	1785	1970	2100	1930

Calculated results for 06/09/2000

Conversion based on THC (Vol %)	0.374531835	0	0.527704	4.032258	10.04566	16.33466	19.58333
Temperature Change (°C)	-10	-7	4	29	40	52	55
Mass flowrate of Air (kg/s)	0.009820627	0.009921	0.009921	0.009921	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	0.0000784	7.84E-05	7.84E-05	7.84E-05	7.84E-05	7.84E-05	7.84E-05
Total mass flow (Kg/s)	0.009999027	0.009999	0.009999	0.009999	0.009999	0.009999	0.009999
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000392	0.000392	0.000392	0.000392	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300	302	304
Conversion based on temp (%)	-3.333333333	-2.333333	1.333333	9.666667	13.33333	17.21854	18.09211
Mols combusted (mol/s)	-1.30667E-05	-9.15E-06	5.23E-06	3.79E-05	5.23E-05	6.75E-05	7.09E-05
Observered reaction rate (mol/sm2)	**-0.000248477**	**-0.000174**	**9.94E-05**	**0.000721**	**0.000994**	**0.001284**	**0.001349**
Density of air at reactor inlet (kg/m3)	1.726778403	1.65574	1.600042	1.492764	1.429546	1.402718	1.373285
Velocity of air through a channel (m/s)	52.44021589	54.69013	56.5939	60.66104	63.34363	64.55512	65.93968
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.09614E-05	3.18E-05	3.26E-05	3.41E-05	3.51E-05	3.55E-05	3.6E-05
Reynolds Number through a channel - calculated at inlet conditions	2924.690872	2843.489	2779.413	2654.836	2580.612	2548.91	2513.956

Based on analyser change

Observed reaction rate (mol/sm2)	**2.79187E-05**	**0**	**3.93E-05**	**0.000301**	**0.000749**	**0.001218**	**0.00146**

Perovskite 8g/l Diesel Inlet temperature - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	LaMnO3
Amount	6 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 06/09/2000

Reactor Pressure (BarG)	2	2
Inlet set temperature (°C)	450	400
Air flowrate (l/min) (Evaluated at ATP)	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6
Actual inlet temp before diesel added (°C)	427	385
Measured wall temp (°C)	427	385
Outlet temp before diesel added (°C)	421	381
Actual inlet temp after diesel added (°C)	456	382
Wall temp after diesel added (°C)	477	387
Outlet temp after diesel added (°C)	479	384
Inlet THC (ppm) (Volume basis)	2410	1785
Outlet (ppm) (Volume basis)	2235	1730

Calculated results for 06/09/2000

Conversion based on THC (Vol %)	7.261410788	3.081232
Temperature Change (°C)	23	2
Mass flowrate of Air (kg/s)	0.009920627	0.009921
Mass flowrate of Fuel (Kg/s)	0.0000784	7.84E-05
Total mass flow (Kg/s)	0.009999027	0.009999
Air to Fuel ratio (mol basis)	872.6800471	872.68
Mols diesel in (mol/s)	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300
Conversion based on temp (%)	7.666666667	0.666667
Mols combusted (mol/s)	3.00533E-05	2.61E-06
Obsevered reaction rate (mol/sm2)	**0.000571496**	**4.97E-05**
Density of air at reactor inlet (kg/m3)	1.435428961	1.5976
Velocity of air through a channel (m/s)	63.08402209	56.68043
Hydrolic mean diameter (m)	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.49956E-05	3.26E-05
Reynolds Number through a channel - calculated at inlet conditions	2587.546892	2776.593

Based on analyser change

Observed reaction rate (mol/sm2)	**0.000541287**	**0.00023**

Perovskite 24g/l Diesel Inlet temperature

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	LaMnO3
Amount	18 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 04/09/2000

Reactor Pressure (BarG)	2	2	2
Inlet set temperature (°C)	500	450	400
Air flowrate (l/min) (Evaluated at ATP)	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	477	433	383
Measured wall temp (°C)	476	431	382
Outlet temp before diesel added (°C)	472	429	382
Actual inlet temp after diesel added (°C)	489	461	385
Wall temp after diesel added (°C)	545	500	394
Outlet temp after diesel added (°C)	548	505	394
Inlet THC (ppm) (Volume basis)	1850	1560	1415
Outlet (ppm) (Volume basis)	1420	1150	1345

Calculated results for 04/09/2000

Conversion based on THC (Vol %)	23.24324324	26.28205	4.946996
Temperature Change (°C)	59	44	9
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	0.0000784	7.84E-05	7.84E-05
Total mass flow (Kg/s)	0.009999027	0.009999	0.009999
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300	300
Conversion based on temp (%)	19.66666667	14.66667	3
Mols combusted (mol/s)	7.70933E-05	5.75E-05	1.18E-05
Obsevered reaction rate (mol/sm2)	**0.001466012**	**0.001093**	**0.000224**
Density of air at reactor inlet (kg/m3)	1.373264714	1.425651	1.590316
Velocity of air through a channel (m/s)	65.93967741	63.5167	56.94004
Hydrolic mean diameter (m)	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.602E-05	3.52E-05	3.27E-05
Reynolds Number through a channel - calculated at inlet conditions	2513.956038	2576.017	2768.183

Based on analyser change

Observed reaction rate (mol/sm2)	**0.001732621**	**0.001959**	**0.000369**

Perovskite 8g/l Diesel Pressure effects - Run 1

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	LaMnO3
Amount	6 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 06/09/2000

Reactor Pressure (BarG)	1.5	2	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	477	478	478	479	480
Measured wall temp (°C)	477	478	478	479	480
Outlet temp before diesel added (°C)	472	468	473	475	480
Actual inlet temp after diesel added (°C)	486	489	492	496	501
Wall temp after diesel added (°C)	518	531	536	551	591
Outlet temp after diesel added (°C)	528	544	550	562	606
Inlet THC (ppm) (Volume basis)	2725	2400	2730	2875	3155
Outlet (ppm) (Volume basis)	2270	1930	2190	2140	2030

Calculated results for 06/09/2000

Conversion based on THC (Vol %)	16.69724771	19.58333	19.78022	25.56522	35.65769
Temperature Change (°C)	42	55	58	66	105
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	0.0000784	7.84E-05	7.84E-05	7.84E-05	7.84E-05
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000392	0.000392	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	14	18.33333	19.33333	22	35
Mols combusted (mol/s)	0.00005488	7.19E-05	7.58E-05	8.62E-05	0.000137
Obsevered reaction rate (mol/sm2)	**0.001043602**	**0.001367**	**0.001441**	**0.00164**	**0.002609**
Density of air at reactor inlet (kg/m3)	1.148910532	1.373265	1.595859	1.814352	2.027961
Velocity of air through a channel (m/s)	78.81608685	65.93968	56.74224	49.90907	44.65207
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.59277E-05	3.6E-05	3.61E-05	3.62E-05	3.64E-05
Reynolds Number through a channel - calculated at inlet conditions	2520.409769	2513.956	2507.547	2499.072	2488.587

Based on analyser change

Observed reaction rate (mol/sm2)	**0.001244663**	**0.00146**	**0.001474**	**0.001906**	**0.002658**

Perovskite 8g/l Diesel Pressure effects - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	LaMnO3
Amount	6 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 06/09/2000

Reactor Pressure (BarG)	1.5	2	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	477	477	480	480	480
Measured wall temp (°C)	477	477	480	480	480
Outlet temp before diesel added (°C)	474	472	475	475	474
Actual inlet temp after diesel added (°C)	485	488	490	495	500
Wall temp after diesel added (°C)	509	517	533	554	576
Outlet temp after diesel added (°C)	513	523	542	565	593
Inlet THC (ppm) (Volume basis)	2200	2630	2840	2840	3060
Outlet (ppm) (Volume basis)	1910	2220	2300	2280	2200

Calculated results for 06/09/2000

Conversion based on THC (Vol %)	13.18181818	15.58935	19.01408	19.71831	28.10458
Temperature Change (°C)	28	35	52	70	93
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	0.0000784	7.84E-05	7.84E-05	7.84E-05	7.84E-05
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000392	0.000392	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	9.333333333	11.66667	17.33333	23.33333	31
Mols combusted (mol/s)	3.65867E-05	4.57E-05	6.79E-05	9.15E-05	0.000122
Obsevered reaction rate (mol/sm2)	**0.000695735**	**0.00087**	**0.001292**	**0.001739**	**0.002311**
Density of air at reactor inlet (kg/m3)	1.150426245	1.375069	1.600042	1.816715	2.030584
Velocity of air through a channel (m/s)	78.71224484	65.85314	56.5939	49.84417	44.59438
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.5897E-05	3.6E-05	3.61E-05	3.62E-05	3.64E-05
Reynolds Number through a channel - calculated at inlet conditions	2522.571124	2516.102	2511.815	2501.183	2490.674

Based on analyser change

Observed reaction rate (mol/sm2)	**0.000982612**	**0.001162**	**0.001417**	**0.00147**	**0.002095**

Perovskite 24g/l Diesel Pressure effects - Run 1

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	LaMnO3
Amount	18 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 04/09/2000

Reactor Pressure (BarG)	1.5	2	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	470	477	478	480	481
Measured wall temp (°C)	468	476	471	479	480
Outlet temp before diesel added (°C)	455	472	473	477	476
Actual inlet temp after diesel added (°C)	483	489	493	497	501
Wall temp after diesel added (°C)	531	545	556	570	591
Outlet temp after diesel added (°C)	532	548	561	579	605
Inlet THC (ppm) (Volume basis)	2170	1850	2480	2750	3020
Outlet (ppm) (Volume basis)	1520	1420	1920	1850	1750

Calculated results for 04/09/2000

Conversion based on THC (Vol %)	29.95391705	23.24324	22.58065	32.72727	42.05298
Temperature Change (°C)	49	59	68	82	104
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	0.0000784	7.84E-05	7.84E-05	7.84E-05	7.84E-05
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000392	0.000392	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	16.33333333	19.66667	22.66667	27.33333	34.66667
Mols combusted (mol/s)	6.40267E-05	7.71E-05	8.89E-05	0.000107	0.000136
Obsevered reaction rate (mol/sm2)	**0.001217535**	**0.001466**	**0.00169**	**0.002038**	**0.002584**
Density of air at reactor inlet (kg/m3)	1.1534697	1.373265	1.593776	1.811996	2.027961
Velocity of air through a channel (m/s)	78.50456082	65.93968	56.81641	49.97397	44.65207
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.58353E-05	3.6E-05	3.61E-05	3.63E-05	3.64E-05
Reynolds Number through a channel - calculated at inlet conditions	2526.909119	2513.956	2505.421	2496.965	2488.587

Based on analyser change

Observed reaction rate (mol/sm2)	**0.002232854**	**0.001733**	**0.001683**	**0.00244**	**0.003135**

Perovskite 24g/l Diesel Pressure effects - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	LaMnO3
Amount	18 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 04/09/2000

Reactor Pressure (BarG)	1.5	2	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	478	478	480	481	482
Measured wall temp (°C)	476	478	479	480	481
Outlet temp before diesel added (°C)	472	477	477	478	475
Actual inlet temp after diesel added (°C)	487	488	491	496	497
Wall temp after diesel added (°C)	532	538	543	578	584
Outlet temp after diesel added (°C)	538	543	547	580	593
Inlet THC (ppm) (Volume basis)	1930	1940	2210	2800	3130
Outlet (ppm) (Volume basis)	1460	1420	1620	1960	1920

Calculated results for 04/09/2000

Conversion based on THC (Vol %)	24.35233161	26.80412	26.69683	30	38.658147
Temperature Change (°C)	51	55	56	84	96
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921	0.0099206
Mass flowrate of Fuel (Kg/s)	0.0000784	7.84E-05	7.84E-05	7.84E-05	0.0000784
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68	872.68005
Mols diesel in (mol/s)	0.000392	0.000392	0.000392	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	17	18.33333	18.66667	28	32
Mols combusted (mol/s)	0.00006664	7.19E-05	7.32E-05	0.00011	0.0001254
Obsevered reaction rate (mol/sm2)	**0.001267231**	**0.001367**	**0.001391**	**0.002087**	**0.0023854**
Density of air at reactor inlet (kg/m3)	1.147398807	1.375069	1.597948	1.814352	2.0384955
Velocity of air through a channel (m/s)	78.91992886	65.85314	56.66807	49.90907	44.421305
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.59585E-05	3.6E-05	3.61E-05	3.62E-05	3.627E-05
Reynolds Number through a channel - calculated at inlet conditions	2518.253483	2516.102	2509.679	2499.072	2496.9652

Based on analyser change

Observed reaction rate (mol/sm2)	**0.001815296**	**0.001998**	**0.00199**	**0.002236**	**0.0028817**

Perovskite 8g/l Diesel Fuel flowrate

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	LaMnO3
Amount	6 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 06/09/2000

Reactor Pressure (BarG)	2	2	2
Inlet set temperature (°C)	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	2.8	4.2	7
Actual inlet temp before diesel added (°C)	478	478	477
Measured wall temp (°C)	478	478	477
Outlet temp before diesel added (°C)	474	474	472
Actual inlet temp after diesel added (°C)	483	483	492
Wall temp after diesel added (°C)	503	508	538
Outlet temp after diesel added (°C)	503	512	552
Inlet THC (ppm) (Volume basis)	1640	2053	3380
Outlet (ppm) (Volume basis)	1570	1885	2844

Calculated results for 06/09/2000

Conversion based on THC (Vol %)	4.268292683	8.183147	15.85799
Temperature Change (°C)	20	29	60
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921
Mass flowrate of Fuel (kg/s)	0.0000392	5.88E-05	0.000098
Total mass flow (Kg/s)	0.009959827	0.009979	0.010019
Air to Fuel ratio (mol basis)	1745.360094	1163.573	698.144
Mols diesel in (mol/s)	0.000196	0.000294	0.00049
Adiabatic temp for 100% conversion (°C)	152	226	372
Conversion based on temp (%)	13.15789474	12.83186	16.12903
Mols combusted (mol/s)	2.57895E-05	3.77E-05	7.9E-05
Obsevered reaction rate (mol/sm2)	**0.000490414**	**0.000717**	**0.001503**
Density of air at reactor inlet (kg/m3)	1.384163641	1.384164	1.367879
Velocity of air through a channel (m/s)	65.42046735	65.42047	66.19928
Hydrolic mean diameter (m)	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.58353E-05	3.58E-05	3.61E-05
Reynolds Number through a channel - calculated at inlet conditions	2526.909119	2526.909	2507.547

Based on analyser change

Observed reaction rate (mol/s/m2)	**0.000159086**	**0.000457**	**0.001478**

Perovskite 24 g/l Diesel Fuel flowrate

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	LaMnO3
Amount	18 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 04/09/2000

Reactor Pressure (BarG)	2	2	2	2
Inlet set temperature (°C)	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	2.8	4.2	5.6	7
Actual inlet temp before diesel added (°C)	476	478	477	479
Measured wall temp (°C)	475	477	476	477
Outlet temp before diesel added (°C)	472	471	472	471
Actual inlet temp after diesel added (°C)	482	486	489	496
Wall temp after diesel added (°C)	503	522	545	580
Outlet temp after diesel added (°C)	503	526	548	591
Inlet THC (ppm) (Volume basis)	1050	1630	1850	2800
Outlet (ppm) (Volume basis)	880	1290	1420	1930

Calculated results for 04/09/2000

Conversion based on THC (Vol %)	16.19047619	20.8589	23.24324	31.07143
Temperature Change (°C)	21	40	59	95
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (kg/s)	0.0000392	5.88E-05	7.84E-05	0.000098
Total mass flow (kg/s)	0.009959827	0.009979	0.009999	0.010019
Air to Fuel ratio (mol basis)	1745.360094	1163.573	872.68	698.144
Mols diesel in (mol/s)	0.000196	0.000294	0.000392	0.00049
Adiabatic temp for 100% conversion (°C)	152	226	300	372
Conversion based on temp (%)	13.81578947	17.69912	19.66667	25.53763
Mols combusted (mol/s)	2.70789E-05	5.2E-05	7.71E-05	0.000125
Obsevered reaction rate (mol/sm2)	**0.000514935**	**0.00099**	**0.001466**	**0.00238**
Density of air at reactor inlet (kg/m3)	1.38599697	1.378693	1.373265	1.360764
Velocity of air through a channel (m/s)	65.33393234	65.68007	65.93968	66.54542
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.58045E-05	3.59E-05	3.6E-05	3.62E-05
Reynolds Number through a channel - calculated at inlet conditions	2529.085798	2520.41	2513.956	2499.072

Based on analyser change

Observed reaction rate (mol/sm2)	**0.000603443**	**0.001166**	**0.001733**	**0.002895**

Perovskite 8g/l Diesel Total mass flow effects 500°C

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel	200

Data on catalysts

Active phase	LaMnO3
Amount	6 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 06/09/2000

Reactor Pressure (BarG)	2	2	2	3.5	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	750	500	250	500	250
Fuel flowrate (ml/min) (Evaluated at ATP)	8.4	5.6	2.8	5.6	2.8
Actual inlet temp before diesel added (°C)	473	478	462	480	463
Measured wall temp (°C)	472	478	462	480	463
Outlet temp before diesel added (°C)	467	468	443	480	444
Actual inlet temp after diesel added (°C)	489	489	480	501	486
Wall temp after diesel added (°C)	510	531	527	591	577
Outlet temp after diesel added (°C)	513	544	519	606	566
Inlet THC (ppm) (Volume basis)	3160	2400	2150	3155	2710
Outlet (ppm) (Volume basis)	2710	1930	1855	2030	2100

Calculated results for 06/09/2000

Conversion based on THC (Vol %)	14.24050633	19.58333	13.72093	35.65769	22.50923
Temperature Change (°C)	24	55	39	105	80
Mass flowrate of Air (kg/s)	0.01488094	0.009921	0.00496	0.009921	0.00496
Mass flowrate of Fuel (Kg/s)	0.0001176	7.84E-05	3.92E-05	7.84E-05	3.92E-05
Total mass flow (Kg/s)	0.01499854	0.009999	0.005	0.009999	0.005
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000588	0.000392	0.000196	0.000392	0.000196
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	8	18.33333	13	35	26.66667
Mols combusted (mol/s)	0.00004704	7.19E-05	2.55E-05	0.000137	5.23E-05
Obsevered reaction rate (mol/sm2)	**0.000894516**	**0.001367**	**0.000485**	**0.002609**	**0.000994**
Density of air at reactor inlet (kg/m3)	1.373264714	1.373265	1.389678	2.027961	2.068039
Velocity of air through a channel (m/s)	98.90951611	65.93968	32.58043	44.65207	21.89336
Hydrolic mean diameter (m)	0.008333333	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.602E-05	3.6E-05	3.57E-05	3.64E-05	3.59E-05
Reynolds Number through a channel - calculated at inlet conditions	31424.45048	2513.956	1266.727	2488.587	1260.205

Based on analyser change

Observed reaction rate (mol/sm2)	**0.001592295**	**0.00146**	**0.000511**	**0.002658**	**0.000839**

Perovskite 8g/l Diesel Total mass flow effects 450°C

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	LaMnO3
Amount	6 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 06/09/2000

Reactor Pressure (BarG)	2	2	2	3.5	3.5	3.5
Inlet set temperature (°C)	450	450	450	450	450	450
Air flowrate (l/min) (Evaluated at ATP)	750	500	250	750	500	250
Fuel flowrate (ml/min) (Evaluated at ATP)	8.4	5.6	2.8	8.4	5.6	2.8
Actual inlet temp before diesel added (°C)	435	427	431	435	433	432
Measured wall temp (°C)	435	427	431	435	433	432
Outlet temp before diesel added (°C)	435	421	427	435	430	429
Actual inlet temp after diesel added (°C)	454	456	453	478	476	461
Wall temp after diesel added (°C)	472	477	479	505	522	501
Outlet temp after diesel added (°C)	475	479	468	520	554	501
Inlet THC (ppm) (Volume basis)	2520	2410	2450	2980	3280	2700
Outlet (ppm) (Volume basis)	2220	2235	2340	2460	2410	2070

Calculated results for 06/09/2000

Conversion based on THC (Vol %)	11.9047619	7.261411	4.489796	17.44966	26.52439	23.33333
Temperature Change (°C)	21	23	15	42	78	40
Mass flowrate of Air (kg/s)	0.01488094	0.009921	0.00496	0.014881	0.009921	0.00496
Mass flowrate of Fuel (Kg/s)	0.0001176	7.84E-05	3.92E-05	0.000118	7.84E-05	3.92E-05
Total mass flow (kg/s)	0.01499854	0.009999	0.005	0.014999	0.009999	0.005
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000588	0.000392	0.000196	0.000588	0.000392	0.000196
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300	300
Conversion based on temp (%)	7	7.666667	5	14	26	13.33333
Mols combusted (mol/s)	0.00004116	3.01E-05	9.8E-06	8.23E-05	0.000102	2.61E-05
Obsevered reaction rate (mol/sm2)	**0.000782701**	**0.000571**	**0.000186**	**0.001565**	**0.001938**	**0.000497**
Density of air at reactor inlet (kg/m3)	1.439377871	1.435429	1.44136	2.090069	2.09565	2.138476
Velocity of air through a channel (m/s)	94.3664281	63.08402	31.41221	64.98779	43.20981	21.17223
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.49328E-05	3.5E-05	3.49E-05	3.57E-05	3.58E-05	3.52E-05
Reynolds Number through a channel - calculated at inlet conditions	3888.298022	2587.547	1297.267	3806.766	2542.255	1288.008

Based on analyser change

Observed reaction rate (mol/s/m2)	**0.001331125**	**0.000541**	**0.000167**	**0.001951**	**0.001977**	**0.00087**

Perovskite 8g/l Diesel Total mass flow effects 400°C

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	LaMnO3
Amount	6 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 06/09/2000

Reactor Pressure (BarG)	2	2	2	3.5	3.5	3.5
Inlet set temperature (°C)	400	400	400	400	400	400
Air flowrate (l/min) (Evaluated at ATP)	750	500	250	750	500	250
Fuel flowrate (ml/min) (Evaluated at ATP)	8.4	5.6	2.8	8.4	5.6	2.8
Actual inlet temp before diesel added (°C)	386	385	391	386	385	390
Measured wall temp (°C)	386	385	391	386	385	390
Outlet temp before diesel added (°C)	386	381	390	385	382	388
Actual inlet temp after diesel added (°C)	381	382	406	399	444	435
Wall temp after diesel added (°C)	383	387	435	451	491	475
Outlet temp after diesel added (°C)	381	384	432	456	488	468
Inlet THC (ppm) (Volume basis)	2090	1785	1770	2720	2230	2200
Outlet (ppm) (Volume basis)	2080	1730	1740	2370	2060	2110

Calculated results for 06/09/2000

Conversion based on THC (Vol %)	0.4784689	3.081232	1.694915	12.86765	7.623318	4.090909
Temperature Change (°C)	0	2	26	57	44	33
Mass flowrate of Air (kg/s)	0.01488094	0.009921	0.00496	0.014881	0.009921	0.00496
Mass flowrate of Fuel (Kg/s)	0.0001176	7.84E-05	3.92E-05	0.000118	7.84E-05	3.92E-05
Total mass flow (kg/s)	0.01499854	0.009999	0.005	0.014999	0.009999	0.005
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000588	0.000392	0.000196	0.000588	0.000392	0.000196
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300	300
Conversion based on temp (%)	0	0.666667	8.666667	19	14.66667	11
Mols combusted (mol/s)	0	2.61E-06	1.7E-05	0.000112	5.75E-05	2.16E-05
Obsevered reaction rate (mol/sm2)	**0**	**4.97E-05**	**0.000323**	**0.002124**	**0.001093**	**0.00041**
Density of air at reactor inlet (kg/m3)	1.600042374	1.5976	1.541131	2.335776	2.189179	2.217008
Velocity of air through a channel (m/s)	84.89084453	56.68043	29.37864	58.15153	41.36373	20.42226
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.25798E-05	3.26E-05	3.34E-05	3.32E-05	3.46E-05	3.43E-05
Reynolds Number through a channel - calculated at inlet conditions	4169.11888	2776.593	1355.601	4094.755	2615.807	1318.783

Based on analyser change

Observed reaction rate (mol/sm2)	**5.34998E-05**	**0.00023**	**6.32E-05**	**0.001439**	**0.000568**	**0.000152**

Perovskite 24g/l Diesel Total mass flow effects 4th Sept 500°C

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	LaMnO3
Amount	18 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 04/09/2000

Reactor Pressure (BarG)	2	2	3.5	3.5	3.5
Inlet set temperature (°C)	500	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	750	500	750	500	250
Fuel flowrate (ml/min) (Evaluated at ATP)	8.4	5.6	8.4	5.6	2.8
Actual inlet temp before diesel added (°C)	475	477	479	481	470
Measured wall temp (°C)	472	476	478	480	465
Outlet temp before diesel added (°C)	464	472	473	476	452
Actual inlet temp after diesel added (°C)	490	489	504	501	486
Wall temp after diesel added (°C)	535	545	607	591	567
Outlet temp after diesel added (°C)	544	548	610	605	568
Inlet THC (ppm) (Volume basis)	2140	1850	3480	3020	2400
Outlet (ppm) (Volume basis)	1820	1420	2350	1750	1360

Calculated results for 04/09/2000

Conversion based on THC (Vol %)	14.95327103	23.24324	32.47126	42.05298	43.33333
Temperature Change (°C)	54	59	106	104	82
Mass flowrate of Air (kg/s)	0.01488094	0.009921	0.014881	0.009921	0.00496
Mass flowrate of Fuel (kg/s)	0.0001176	7.84E-05	0.000118	7.84E-05	3.92E-05
Total mass flow (Kg/s)	0.01499854	0.009999	0.014999	0.009999	0.005
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000588	0.000392	0.000588	0.000392	0.000196
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300
Conversion based on temp (%)	18	19.66667	35.33333	34.66667	27.33333
Mols combusted (mol/s)	0.00010584	7.71E-05	0.000208	0.000136	5.36E-05
Obsevered reaction rate (mol/sm2)	**0.002012661**	**0.001466**	**0.003951**	**0.002584**	**0.001019**
Density of air at reactor inlet (kg/m3)	1.371464892	1.373265	2.020131	2.027961	2.068039
Velocity of air through a channel (m/s)	99.03931862	65.93968	67.2377	44.65207	21.89336
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.60507E-05	3.6E-05	3.65E-05	3.64E-05	3.59E-05
Reynolds Number through a channel - calculated at inlet conditions	3767.722262	2513.956	3723.53	2488.587	1260.205

Based on analyser change

Observed reaction rate (mol/sm2)	**0.001671992**	**0.001733**	**0.003631**	**0.003135**	**0.001615**

Perovskite 24g/l Diesel Total mass flow effects 4th Sept 450°C

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	LaMnO3
Amount	18 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 04/09/2000

Reactor Pressure (BarG)	2	2	2	3.5	3.5	3.5
Inlet set temperature (°C)	450	450	450	450	450	450
Air flowrate (l/min) (Evaluated at ATP)	750	500	250	750	500	250
Fuel flowrate (ml/min) (Evaluated at ATP)	8.4	5.6	2.8	8.4	5.6	2.8
Actual inlet temp before diesel added (°C)	433	433	435	435	437	435
Measured wall temp (°C)	432	431	436	434	437	436
Outlet temp before diesel added (°C)	431	429	436	431	437	436
Actual inlet temp after diesel added (°C)	463	461	455	482	488	455
Wall temp after diesel added (°C)	493	500	509	553	538	512
Outlet temp after diesel added (°C)	500	505	515	566	538	522
Inlet THC (ppm) (Volume basis)	1680	1560	1490	3070	2340	1770
Outlet (ppm) (Volume basis)	1260	1150	1115	1980	1430	1108

Calculated results for 04/09/2000

Conversion based on THC (Vol %)	25	26.28205	25.16779	35.50489	38.88889	37.40113
Temperature Change (°C)	37	44	60	84	70	67
Mass flowrate of Air (kg/s)	0.01488094	0.009921	0.00496	0.014881	0.009921	0.00496
Mass flowrate of Fuel (kg/s)	0.0001176	7.84E-05	3.92E-05	0.000118	7.84E-05	3.92E-05
Total mass flow (kg/s)	0.01499854	0.009999	0.005	0.014999	0.009999	0.005
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000588	0.000392	0.000196	0.000588	0.000392	0.000196
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300	300
Conversion based on temp (%)	12.33333333	14.66667	20	28	23.33333	22.33333
Mols combusted (mol/s)	0.00007252	5.75E-05	3.92E-05	0.000165	9.15E-05	4.38E-05
Obsevered reaction rate (mol/sm2)	**0.001379045**	**0.001093**	**0.000745**	**0.003131**	**0.001739**	**0.000832**
Density of air at reactor inlet (kg/m3)	1.421776783	1.425651	1.437401	2.078995	2.118275	2.156101
Velocity of air through a channel (m/s)	95.53485073	63.5167	31.49874	65.33393	42.74829	20.99916
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.52147E-05	3.52E-05	3.5E-05	3.58E-05	3.54E-05	3.5E-05
Reynolds Number through a channel - calculated at inlet conditions	3857.16624	2576.017	1294.935	3793.629	2560.109	1294.935

Based on analyser change

Observed reaction rate (mol/sm2)	**0.002795362**	**0.001959**	**0.000938**	**0.00397**	**0.002899**	**0.001394**

Perovskite 24g/l Diesel Total mass flow effects 4th Sept 400°C

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel fuel (g/mol)	200

Data on catalysts

Active phase	LaMnO3
Amount	18 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 04/09/2000

Reactor Pressure (BarG)	2	2	2	3.5	3.5	3.5
Inlet set temperature (°C)	400	400	400	400	400	400
Air flowrate (l/min) (Evaluated at ATP)	750	500	250	750	500	250
Fuel flowrate (ml/min) (Evaluated at ATP)	8.4	5.6	2.8	8.4	5.6	2.8
Actual inlet temp before diesel added (°C)	383	383	391	385	388	392
Measured wall temp (°C)	384	382	391	384	388	391
Outlet temp before diesel added (°C)	382	382	391	380	385	390
Actual inlet temp after diesel added (°C)	383	385	410	403	435	436
Wall temp after diesel added (°C)	384	394	443	467	465	472
Outlet temp after diesel added (°C)	383	394	439	486	491	472
Inlet THC (ppm) (Volume basis)	870	1415	1010	1890	1815	2010
Outlet (ppm) (Volume basis)	790	1345	965	1435	1335	1610

Calculated results for 04/09/2000

Conversion based on THC (Vol %)	9.195402299	4.946996	4.455446	24.07407	26.44628	19.9005
Temperature Change (°C)	0	9	29	83	56	36
Mass flowrate of Air (kg/s)	0.01488094	0.009921	0.00496	0.014881	0.009921	0.00496
Mass flowrate of Fuel (kg/s)	0.0001176	7.84E-05	3.92E-05	0.000118	7.84E-05	3.92E-05
Total mass flow (kg/s)	0.01499854	0.009999	0.005	0.014999	0.009999	0.005
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000588	0.000392	0.000196	0.000588	0.000392	0.000196
Adiabatic temp for 100% conversion (°C)	300	300	300	300	300	300
Conversion based on temp (%)	0	3	9.666667	27.66667	18.66667	12
Mols combusted (mol/s)	0	1.18E-05	1.89E-05	0.000163	7.32E-05	2.35E-05
Obsevered reaction rate (mol/sm2)	**0**	**0.000224**	**0.00036**	**0.003094**	**0.001391**	**0.000447**
Density of air at reactor inlet (kg/m3)	1.595164196	1.590316	1.532105	2.321955	2.217008	2.213881
Velocity of air through a channel (m/s)	85.15044956	56.94004	29.55171	58.49767	40.84452	20.45111
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.26459E-05	3.27E-05	3.35E-05	3.33E-05	3.43E-05	3.44E-05
Reynolds Number through a channel - calculated at inlet conditions	4160.673077	2768.183	1350.355	4078.719	2637.565	1317.562

Based on analyser change

Observed reaction rate (mol/sm2)	**0.001028179**	**0.000369**	**0.000166**	**0.002692**	**0.001971**	**0.000742**

APPENDIX I

Degussa Diesel Inlet temperature - Run 1

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Moleculare weight diesel fuel (g/mol)	200

Data on catalysts

Active phase	Degussa (Pt)
Amount	3 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 09/09/2000

Reactor Pressure (BarG)	2	2	2
Inlet set temperature (°C)	350	400	450
Air flowrate (l/min) (Evaluated at ATP)	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	337	381	429
Measured wall temp (°C)	337	380	429
Outlet temp before diesel added (°C)	331	370	422
Actual inlet temp after diesel added (°C)	333	379	455
Wall temp after diesel added (°C)	479	569	617
Outlet temp after diesel added (°C)	466	515	595
Inlet THC (ppm) (Volume basis)	1550	2000	2150
Outlet (ppm) (Volume basis)	800	1035	965

Calculated results for 09/08/2000

Conversion based on THC (Vol %)	48.38709677	48.25	55.11628
Temperature Change (°C)	133	136	140
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921
Mass flowrate of Fuel (kg/s)	0.0000784	7.84E-05	7.84E-05
Total mass flow (kg/s)	0.009999027	0.009999	0.009999
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300	300
Conversion based on temp (%)	44.33333333	45.33333	46.66667
Mols combusted (mol/s)	0.000173787	0.000178	0.000183
Obsevered reaction rate (mol/sm2)	**0.003304739**	**0.003379**	**0.003479**
Density of air at reactor inlet (kg/m3)	1.726778403	1.60495	1.437401
Velocity of air through a channel (m/s)	52.44021589	56.42083	62.99749
Hydrolic mean diameter (m)	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.09614E-05	3.25E-05	3.5E-05
Reynolds Number through a channel - calculated at inlet conditions	2924.690872	2785.075	2589.87

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.003606919**	**0.003597**	**0.004109**

Degussa Diesel Inlet temperature - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight diesel fuel	200

Data on catalysts

Active phase	Degussa (Pt)
Amount	3 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 09/09/2000

Reactor Pressure (BarG)	2	2	2	2
Inlet set temperature (°C)	350	400	450	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	340	388	432	480
Measured wall temp (°C)	340	388	432	480
Outlet temp before diesel added (°C)	340	388	427	476
Actual inlet temp after diesel added (°C)	335	384	459	490
Wall temp after diesel added (°C)	496	573	647	677
Outlet temp after diesel added (°C)	480	555	609	667
Inlet THC (ppm) (Volume basis)	1850	1970	1956	2950
Outlet (ppm) (Volume basis)	970	900	760	1090

Calculated results for 09/09/2000

Conversion based on THC (Vol %)	47.56756757	54.31472	61.14519	63.05085
Temperature Change (°C)	145	171	150	177
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (kg/s)	0.0000784	7.84E-05	7.84E-05	7.84E-05
Total mass flow (kg/s)	0.009999027	0.009999	0.009999	0.009999
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000392	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	48.33333333	57	50	59
Mols combusted (mol/s)	0.000189467	0.000223	0.000196	0.000231
Obsevered reaction rate (mol/sm2)	**0.003602911**	**0.004249**	**0.003727**	**0.004398**
Density of air at reactor inlet (kg/m3)	1.721098211	1.592736	1.429546	1.371465
Velocity of air through a channel (m/s)	52.61328591	56.8535	63.34363	66.02621
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.10301E-05	3.27E-05	3.51E-05	3.61E-05
Reynolds Number through a channel - calculated at inlet conditions	2918.218244	2770.978	2580.612	2511.815

Based on analyser change

Observed rate of reaction (mol/sm2)	**0.003545829**	**0.004049**	**0.004558**	**0.0047**

Degussa Diesel Pressure effects - Run 1

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of diesel (g/mol)	200

Data on catalysts

Active phase	Degussa (Pt)
Amount	3 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 09/09/2000

Reactor Pressure (BarG)	1.5	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	477	477	477	477
Measured wall temp (°C)	477	477	477	477
Outlet temp before diesel added (°C)	468	468	469	468
Actual inlet temp after diesel added (°C)	485	490	496	500
Wall temp after diesel added (°C)	656	683	684	722
Outlet temp after diesel added (°C)	641	664	676	710
Inlet THC (ppm) (Volume basis)	2800	2950	3440	3450
Outlet (ppm) (Volume basis)	1110	1050	1500	820

Calculated results for 09/09/2000

Conversion based on THC (Vol %)	60.35714286	64.40678	56.39535	76.23188
Temperature Change (°C)	156	174	180	210
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (kg/s)	0.0000784	7.84E-05	7.84E-05	7.84E-05
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000392	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	52	58	60	70
Mols combusted (mol/s)	0.00020384	0.000227	0.000235	0.000274
Obsevered reaction rate (mol/sm2)	**0.003876235**	**0.004323**	**0.004473**	**0.005218**
Density of air at reactor inlet (kg/m3)	1.150426245	1.600042	1.814352	2.030584
Velocity of air through a channel (m/s)	78.71224484	56.5939	49.90907	44.59438
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.5897E-05	3.61E-05	3.62E-05	3.64E-05
Reynolds Number through a channel - calculated at inlet conditions	2522.571124	2511.815	2499.072	2490.674

Based Analyser change

Obsereved rate of reaction (mol/s.m2)	**0.004499202**	**0.004801**	**0.004204**	**0.005683**

Degussa Diesel Pressure effects - Run 2

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of Diesel fuel (g/mol)	200

Data on catalysts

Active phase	Degussa (Pt)
Amount	3 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 09/09/2000

Reactor Pressure (BarG)	2	2.5	3	3.5
Inlet set temperature (°C)	500	500	500	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	480	480	481	481
Measured wall temp (°C)	480	480	481	481
Outlet temp before diesel added (°C)	476	477	477	476
Actual inlet temp after diesel added (°C)	490	493	495	498
Wall temp after diesel added (°C)	677	697	678	725
Outlet temp after diesel added (°C)	667	681	688	703
Inlet THC (ppm) (Volume basis)	2950	3300	2900	3481
Outlet (ppm) (Volume basis)	1090	1355	990	1250

Calculated results for 09/09/2000

Conversion based on THC (Vol %)	63.05084746	58.93939	65.86207	64.09078
Temperature Change (°C)	177	188	193	205
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (kg/s)	0.0000784	7.84E-05	7.84E-05	7.84E-05
Air to Fuel ratio (mass basis)	872.6800471	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000392	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	59	62.66667	64.33333	68.33333
Mols combusted (mol/s)	0.00023128	0.000246	0.000252	0.000268
Obsevered reaction rate (mol/sm2)	**0.004398036**	**0.004671**	**0.004796**	**0.005094**
Density of air at reactor inlet (kg/m3)	1.371464892	1.593776	1.816715	2.035852
Velocity of air through a channel (m/s)	66.02621242	56.81641	49.84417	44.47899
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.60507E-05	3.61E-05	3.62E-05	3.63E-05
Reynolds Number through a channel - calculated at inlet conditions	2511.814842	2505.421	2501.183	2494.863

Based on Analyser change

Obsevrved reaction rate (mol/sm2)	**0.004699999**	**0.004394**	**0.00491**	**0.004778**

APPENDIX J

Blank Inlet temperature - Petrol

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Petrol (kg/m3)	733
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of Petrol (g/mol)	98

Data on catalysts

Active phase	-
Amount	-
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 22/09/2000

Reactor Pressure (BarG)	2	2	2	2
Inlet set temperature (°C)	300	400	450	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	6.1	6.1	6.1	6.1
Actual inlet temp before petrol added (°C)	282	388	431	476
Measured wall temp (°C)	283	388	431	476
Outlet temp before petrol added (°C)	288	384	423	476
Actual inlet temp after petrol added (°C)	281	383	430	474
Wall temp after petrol added (°C)	283	385	431	476
Outlet temp after petrol added (°C)	287	385	433	478
Inlet THC (ppm) (Volume basis)	N/A	N/A	N/A	N/A
Outlet (ppm) (Volume basis)	N/A	N/A	N/A	N/A

Calculated results for 22/09/2000

Conversion based on THC (Vol %)	#VALUE!	#VALUE!	#VALUE!	#VALUE!
Temperature Change (°C)	6	2	3	4
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	7.45217E-05	7.45E-05	7.45E-05	7.45E-05
Total mass flow (Kg/s)	0.009995148	0.009995	0.009995	0.009995
Air to Fuel ratio (mol basis)	449.8675109	449.8675	449.8675	449.8675
Mols petrol in (mol/s)	0.000760425	0.00076	0.00076	0.00076
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	2	0.666667	1	1.333333
Mols combusted (mol/s)	1.52085E-05	5.07E-06	7.6E-06	1.01E-05
Obsevered reaction rate (mol/sm2)	**0.000289206**	**9.64E-05**	**0.000145**	**0.000193**
Density of air at reactor inlet (kg/m3)	1.888858686	1.595164	1.488517	1.40084
Velocity of air through a channel (m/s)	47.94039538	56.76697	60.83411	64.64165
Hydrolic mean diameter (m)	0.008333333	0.008333	0.008333	0.008333
Viscosity of air at inlet conditions (N.s/m2)	2.91346E-05	3.26E-05	3.42E-05	3.56E-05
Reynolds Number through a channel - calculated at inlet conditions	25900.65406	23114.85	22082.25	21222.39

Based Analyser change

Obsereved rate of reaction (mol/s.m2)	**#VALUE!**	**#VALUE!**	**#VALUE!**	**#VALUE!**

Blank Inlet temperature Diesel

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Density of liquid Diesel fuel (kg/m3)	840
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of Diesel (g/mol)	200

Data on catalysts

Active phase	-
Amount	-
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 09/09/2000

Reactor Pressure (BarG)	2	2	2	2
Inlet set temperature (°C)	350	400	450	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (ml/min) (Evaluated at ATP)	5.6	5.6	5.6	5.6
Actual inlet temp before diesel added (°C)	332	379	424	471
Measured wall temp (°C)	332	379	424	471
Outlet temp before diesel added (°C)	318	366	411	456
Actual inlet temp after diesel added (°C)	332	381	454	489
Wall temp after diesel added (°C)	332	381	473	490
Outlet temp after diesel added (°C)	323	379	468	500
Inlet THC (ppm) (Volume basis)	2270	1900	1924	2310
Outlet (ppm) (Volume basis)	2100	1920	1660	2080

Calculated results for 09/09/2000

Conversion based on THC (Vol %)	7.488986784	-1.05263	13.72141	9.95671
Temperature Change (°C)	-9	-2	14	11
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	0.0000784	7.84E-05	7.84E-05	7.84E-05
Total mass flow (Kg/s)	0.009999027	0.009999	0.009999	0.009999
Air to Fuel ratio (mol basis)	872.6800471	872.68	872.68	872.68
Mols diesel in (mol/s)	0.000392	0.000392	0.000392	0.000392
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	-3	-0.66667	4.666667	3.666667
Mols combusted (mol/s)	-0.00001176	-2.6E-06	1.83E-05	1.44E-05
Obsevered reaction rate (mol/sm2)	**-0.00022363**	**-5E-05**	**0.000348**	**0.000273**
Density of air at reactor inlet (kg/m3)	1.729632582	1.600042	1.439378	1.373265
Velocity of air through a channel (m/s)	52.35368088	56.5939	62.91095	65.93968
Hydrolic mean diameter (m)	0.008333333	0.008333	0.008333	0.008333
Viscosity of air at inlet conditions (N.s/m2)	3.09271E-05	3.26E-05	3.49E-05	3.6E-05
Reynolds Number through a channel - calculated at inlet conditions	24399.51635	23161.77	21601.66	20949.63

Based Analyser change

Obsereved rate of reaction (mol/s.m2)	**0.00011165**	**-1.6E-05**	**0.000205**	**0.000148**

APPENDIX K

Platinum 8 g/l Methane Inlet temperature

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of Methane (g/mol)	16

Data on catalysts

Active phase	LaMnO3
Amount	18 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 02/10/2000

Reactor Pressure (BarG)	2	2	2	2
Inlet set temperature (°C)	350	400	450	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (l/min) (Evaluated at ATP)	9	9	9	9
Actual inlet temp before Methane added (°C)	335	382	428	475
Measured wall temp (°C)	335	382	427	474
Outlet temp before Methane added (°C)	327	372	417	462
Actual inlet temp after Methane added (°C)	333	380	425	471
Wall temp after Methane added (°C)	333	380	425	471
Outlet temp after Methane added (°C)	326	370	415	460
Inlet THC (ppm) (Volume basis)	6090	6010	6040	6120
Outlet (ppm) (Volume basis)	6090	6090	6090	6120

Calculated results for 02/10/2000

Conversion based on THC (Vol %)	0	-1.33111	-0.82781	0
Temperature Change (°C)	-7	-10	-10	-11
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	9.85221E-05	9.85E-05	9.85E-05	9.85E-05
Total mass flow (Kg/s)	0.010019149	0.010019	0.010019	0.010019
Air to Fuel ratio (mol basis)	193.7829097	193.7829	193.7829	193.7829
Mols Methane in (mol/s)	0.00615763	0.006158	0.006158	0.006158
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	-2.333333333	-3.33333	-3.33333	-3.66667
Mols combusted (mol/s)	-0.000143678	-0.00021	-0.00021	-0.00023
Obsevered reaction rate (mol/sm2)	**-0.002732191**	**-0.0039**	**-0.0039**	**-0.00429**
Density of air at reactor inlet (kg/m3)	1.726778403	1.602493	1.49918	1.406489
Velocity of air through a channel (m/s)	52.44021589	56.50736	60.40144	64.38205
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.09614E-05	3.25E-05	3.4E-05	3.55E-05
Reynolds Number through a channel - calculated at inlet conditions	2924.690872	2782.24	2662.333	2553.373

Based on analyser change

Observed reaction rate (mol/sm2)	**0**	**-0.00156**	**-0.00097**	**0**

Perovskite 24 g/l Methane Inlet temperature

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of Methane (g/mol)	16

Data on catalysts

Active phase	LaMnO3
Amount	18 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 02/10/2000

Reactor Pressure (BarG)	2	2	2	2
Inlet set temperature (°C)	350	400	450	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (l/min) (Evaluated at ATP)	9	9	9	9
Actual inlet temp before Methane added (°C)	330	382	429	476
Measured wall temp (°C)	330	381	428	474
Outlet temp before Methane added (°C)	318	370	419	462
Actual inlet temp after Methane added (°C)	328	378	425	470
Wall temp after Methane added (°C)	329	377	424	469
Outlet temp after Methane added (°C)	321	369	416	459
Inlet THC (ppm) (Volume basis)	7600	6520	6370	6180
Outlet (ppm) (Volume basis)	7600	6620	6340	6280

Calculated results for 02/10/2000

Conversion based on THC (Vol %)	0	-1.53374	0.470958	-1.61812
Temperature Change (°C)	-7	-9	-9	-11
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	9.85221E-05	9.85E-05	9.85E-05	9.85E-05
Total mass flow (Kg/s)	0.010019149	0.010019	0.010019	0.010019
Air to Fuel ratio (mol basis)	193.7829097	193.7829	193.7829	193.7829
Mols Methane in (mol/s)	0.00615763	0.006158	0.006158	0.006158
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	-2.333333333	-3	-3	-3.66667
Mols combusted (mol/s)	-0.000143678	-0.00018	-0.00018	-0.00023
Obsevered reaction rate (mol/sm2)	**-0.002732191**	**-0.00351**	**-0.00351**	**-0.00429**
Density of air at reactor inlet (kg/m3)	1.74114428	1.607416	1.49918	1.408382
Velocity of air through a channel (m/s)	52.00754084	56.33429	60.40144	64.29551
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.07893E-05	3.25E-05	3.4E-05	3.54E-05
Reynolds Number through a channel - calculated at inlet conditions	2941.045967	2787.917	2662.333	2555.613

Based on analyser change

Observed reaction rate (mol/sm2)	**0**	**-0.0018**	**0.000551**	**-0.00189**

Degussa Methane Inlet temperature

Constants for calculations

Atmospheric pressure (Bar)	1
Atmospheric temperature (°C)	20
Molecular weight of Air (g/mol)	29
Gas constant (J/mol.K)	8.314
Molecular weight of Methane (g/mol)	16

Data on catalysts

Active phase	LaMnO3
Amount	18 wt %
Calcination temp (°C)	800
Cell type	square
Cells per square inch	400
Length of a section (mm)	20
Diameter of a section (mm)	15
No of sections	6
Length of a channel (mm)	1
Number of cells in sample	110
Geometric surface area of sample (m2)	0.052587106

Data for 02/10/2000

Reactor Pressure (BarG)	2	2	2	2
Inlet set temperature (°C)	350	400	450	500
Air flowrate (l/min) (Evaluated at ATP)	500	500	500	500
Fuel flowrate (l/min) (Evaluated at ATP)	9	9	9	9
Actual inlet temp before Methane added (°C)	335	381	428	474
Measured wall temp (°C)	335	381	427	473
Outlet temp before Methane added (°C)	329	370	417	460
Actual inlet temp after Methane added (°C)	332	379	424	470
Wall temp after Methane added (°C)	333	379	424	469
Outlet temp after Methane added (°C)	328	371	416	460
Inlet THC (ppm) (Volume basis)	6150	6060	6080	6030
Outlet (ppm) (Volume basis)	6160	6060	6010	6050

Calculated results for 02/10/2000

Conversion based on THC (Vol %)	-0.162601626	0	1.151316	-0.33167
Temperature Change (°C)	-4	-8	-8	-10
Mass flowrate of Air (kg/s)	0.009920627	0.009921	0.009921	0.009921
Mass flowrate of Fuel (Kg/s)	9.85221E-05	9.85E-05	9.85E-05	9.85E-05
Total mass flow (Kg/s)	0.010019149	0.010019	0.010019	0.010019
Air to Fuel ratio (mol basis)	193.7829097	193.7829	193.7829	193.7829
Mols Methane in (mol/s)	0.00615763	0.006158	0.006158	0.006158
Adiabatic temp for 100% conversion (°C)	300	300	300	300
Conversion based on temp (%)	-1.333333333	-2.66667	-2.66667	-3.33333
Mols combusted (mol/s)	-8.21017E-05	-0.00016	-0.00016	-0.00021
Obsevered reaction rate (mol/sm2)	**-0.001561252**	**-0.00312**	**-0.00312**	**-0.0039**
Density of air at reactor inlet (kg/m3)	1.729632582	1.60495	1.501331	1.408382
Velocity of air through a channel (m/s)	52.35368088	56.42083	60.3149	64.29551
Hydrolic mean diameter (m)	0.001	0.001	0.001	0.001
Viscosity of air at inlet conditions (N.s/m2)	3.09271E-05	3.25E-05	3.4E-05	3.54E-05
Reynolds Number through a channel - calculated at inlet conditions	2927.941961	2785.075	2664.845	2555.613

Based on analyser change

Observed reaction rate (mol/sm2)	**-0.000190397**	**0**	**0.001348**	**-0.00039**